SURFACE AND SUBSURFACE FLOW AND CONTAMINANT TRANSPORT MODELING IN LOWER ALTAMAHA WATERSHED

by

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Orhan Gunduz and Mustafa M. Aral

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List of Symbols

\[ A \quad \text{: Active cross-sectional area of channel flow (L}^2\text{)} \]
\[ A_o \quad \text{: Inactive cross-sectional area (off-channel storage) (L}^2\text{)} \]
\[ B \quad \text{: Active cross-sectional top width (L)} \]
\[ B_o \quad \text{: Inactive cross-sectional top width (L)} \]
\[ C \quad \text{: Specific moisture capacity in the unsaturated zone (L}^{-1}\text{)} \]
\[ c_1 \quad \text{: Unit system dependent constant in Manning’s equation (-)} \]
\[ C_{gd} \quad \text{: Specified contaminant concentration in groundwater (ML}^{-3}\text{)} \]
\[ C_g \quad \text{: Vertically-averaged contaminant concentration in groundwater (ML}^{-3}\text{)} \]
\[ C_g^\hat{\quad} \quad \text{: Approximate vertically-averaged contaminant concentration in groundwater (ML}^{-3}\text{)} \]
\[ C_{g0} \quad \text{: Initial contaminant concentration in groundwater (ML}^{-3}\text{)} \]
\[ C_i \quad \text{: Contaminant concentration in infiltrating water (ML}^{-3}\text{)} \]
\[ C_o \quad \text{: Contaminant concentration in overland inflow to the river channel (ML}^{-3}\text{)} \]
\[ C_r \quad \text{: Contaminant concentration in river channel (ML}^{-3}\text{)} \]
\[ C_{r0} \quad \text{: Initial contaminant concentration in river channel (ML}^{-3}\text{)} \]
\[ C_{ru} \quad \text{: Upstream boundary condition contaminant concentration in river channel (ML}^{-3}\text{)} \]
\[ C_v \quad \text{: Contaminant concentration in the inflowing stream of variable boundary condition in groundwater (ML}^{-3}\text{)} \]
\[ C_w \quad \text{: Contaminant concentration in point source (ML}^{-3}\text{)} \]
\[ d \quad \text{: Water depth in the river channel (L)} \]
\[ D \quad \text{: Hydrodynamic dispersion coefficient in groundwater (L}^2\text{T}^{-1}\text{)} \]
\[ D_l \quad \text{: Longitudinal dispersion coefficient in river channel (L}^2\text{T}^{-1}\text{)} \]
\[ D_m \quad \text{: Molecular diffusion coefficient (L}^2\text{T}^{-1}\text{)} \]
\[ D_{sed} \quad \text{: Vertical dispersion coefficient in the channel bed (L}^2\text{T}^{-1}\text{)} \]
\[ f \quad \text{: Arbitrary function (-)} \]
\[ g \quad \text{: Gravitational acceleration (LT}^{-2}\text{)} \]
\[ g_x \quad \text{: The x-coordinate of the parametric equation defining the river in domain (-)} \]
\[ g_y \quad \text{: The y-coordinate of the parametric equation defining the river in domain (-)} \]
\[ h_d \quad \text{: Downstream boundary condition water surface elevation in river (L)} \]


\( h_g \) : Vertically-averaged groundwater hydraulic head above a datum (L)
\( h_{g0} \) : Initial groundwater head (L)
\( h_{gD} \) : Specified head boundary condition value in groundwater (L)
\( \hat{h}_g \) : Approximate groundwater hydraulic head above a datum (L)
\( \left( \hat{h}_g \right)_{avg} \) : Element average approximate groundwater head above a datum (L)
\( h_o \) : Overland flow water surface elevation (stage) above a datum (L)
\( h_{o0} \) : Initial overland flow water surface elevation (stage) above a datum (L)
\( h_{oD} \) : Initial overland flow water surface elevation (stage) above a datum (L)
\( h_r \) : Channel flow water surface elevation (stage) above a datum (L)
\( h_{r0} \) : Initial water surface elevation in channel (L)
\( h_r \) : Total head loss in a junction (L)
\( h_u \) : Upstream boundary condition water surface elevation in river channel (L)
\( H \) : Heaviside step function (-)
\( I \) : Infiltration rate (LT\(^{-1}\))
\( k \) : Decay coefficient of contaminant (T\(^{-1}\))
\( K \) : Channel conveyance (L\(^3\)T\(^{-1}\))
\( K_d \) : Partitioning coefficient (L\(^3\)M\(^{-1}\))
\( K_{ec} \) : Contraction/expansion coefficient (-)
\( K_g \) : Saturated hydraulic conductivity in groundwater (LT\(^{-1}\))
\( K_o \) : Diffusion coefficients in overland flow (L\(^2\)T\(^{-1}\))
\( K_r \) : Saturated hydraulic conductivity of channel bottom sediments (LT\(^{-1}\))
\( K_v \) : Unsaturated hydraulic conductivity in vertical direction (LT\(^{-1}\))
\( K_w \) : Biodegradation rate constant for contaminant (T\(^{-1}\))
\( M \) : Mass loading (MT\(^{-1}\))
\( M_{L1} \) : Momentum flux due to lateral seepage inflow/outflow (L\(^3\)T\(^{-2}\))
\( M_{L2} \) : Momentum flux due to lateral overland inflow/outflow (L\(^3\)T\(^{-2}\))
\( m \) : Constant in kinematic wave equation (-)
\( m_r \) : Thickness of the channel bottom sediments (L)
\( m_e \) : Empirical constant in van Genuchten model (-)
\( n \) : Porosity of the medium (-)
\( n_c \) : Manning’s roughness coefficient in channel (L\(^{-1/3}\)T)
\( n_o \) : Manning’s roughness coefficient over land surface (L\(^{-1/3}\)T)
\( n_{sed} \) : Porosity of the channel bottom sediment (-)
\( n_r \) : Number of river channels in the domain (-)
\( n_v \) : Empirical constant in van Genuchten model (-)
\( n_w \) : Number of wells in the domain (-)

\( N \) : Total number of nodes in the entire channel network or in groundwater flow domain (-)

\( N_i \) : \( i \)th weighing function (-)

\( N_j \) : \( j \)th shape function (-)

\( N_k \) : Number of nodes in channel \( k \) (-)

\( q \) : Darcy flux \((L^3T^{-1})\)

\( q_{L1} \) : Lateral seepage inflow/outflow per channel length \((L^3T^{-1})\)

\( q_{L2} \) : Lateral overland inflow/outflow per channel length \((L^3T^{-1})\)

\( q_C \) : Head-dependent boundary condition flux value \((L^3T^{-1})\)

\( q_N \) : Specified flux boundary condition value \((L^3T^{-1})\)

\( q_v \) : Volumetric inflowing flux rate of variable boundary condition \((L^2T^{-1})\)

\( Q \) : Channel discharge \((L^3T^{-1})\)

\( Q_0 \) : Initial channel discharge \((L^3T^{-1})\)

\( Q_d \) : Downstream boundary condition discharge \((L^3T^{-1})\)

\( Q_u \) : Upstream boundary condition discharge \((L^3T^{-1})\)

\( Q_w \) : Point source (i.e., well) strength \((L^3T^{-1})\)

\( R \) : Precipitation rate \((LT^{-1})\)

\( \tilde{R} \) : Residual in the Galerkin method (variable in each model)

\( R_d \) : Retardation coefficient (-)

\( R_h \) : Hydraulic radius \((L)\)

\( s \) : Scale parameter in under-relaxation coefficient (-)

\( s_c \) : Sinuosity factor for continuity equation (-)

\( s_m \) : Sinuosity factor for momentum equation (-)

\( S_{ec} \) : Contraction/expansion slope (-)

\( S_e \) : Effective saturation content (-)

\( S_f \) : Channel/floodplain boundary friction slope (-)

\( S_s \) : Specific storage coefficient \((L^3T^{-1})\)

\( S_w \) : Degree of saturation in unsaturated zone (-)

\( S_y \) : Specific yield of unconfined aquifer (-)

\( t \) : Time coordinate \((T)\)

\( u \) : Parameter of the parametric equation defining sources and sinks (-)

\( v \) : Pore-water velocity in groundwater \((LT^{-1})\)

\( V \) : Flow velocity in the river channel \((LT^{-1})\)

\( V^* \) : Shear velocity in the river channel \((LT^{-1})\)

\( w_r \) : Wetted perimeter of channel bed \((L)\)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$</td>
<td>Global spatial coordinate in longitudinal direction (L)</td>
</tr>
<tr>
<td>$y$</td>
<td>Global spatial coordinate in transverse direction (L)</td>
</tr>
<tr>
<td>$z$</td>
<td>Global spatial coordinate in vertical direction (L)</td>
</tr>
<tr>
<td>$z_b$</td>
<td>Top elevation of bottom impervious layer above a datum (L)</td>
</tr>
<tr>
<td>$z_g$</td>
<td>Ground surface elevation above a datum (L)</td>
</tr>
<tr>
<td>$z_r$</td>
<td>Bottom elevation of channel bed above a datum (L)</td>
</tr>
<tr>
<td>$z_{wt}$</td>
<td>Water table elevation above a datum (L)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>Weighing coefficient (-)</td>
</tr>
<tr>
<td>$\alpha_c$</td>
<td>A weighing parameter in Newton-Raphson method used to evaluate the first estimate of the unknown variables (-)</td>
</tr>
<tr>
<td>$\alpha_k$</td>
<td>A constant in kinematic wave equation (L$^{1/3}$T$^{-1}$)</td>
</tr>
<tr>
<td>$\alpha_L$</td>
<td>Longitudinal dispersivity of porous medium (L)</td>
</tr>
<tr>
<td>$\alpha_T$</td>
<td>Transverse dispersivity of porous medium (L)</td>
</tr>
<tr>
<td>$\alpha_g$</td>
<td>Empirical constant in van Genuchten model (-)</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Momentum correction coefficient for non-uniform velocity distribution (-)</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Kronecker delta (-) or Dirac delta function (argument$^{-1}$)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Iteration-dependent under-relaxation coefficient (-)</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>Maximum change in hydraulic head for all nodes between two iterations (L)</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Local transverse coordinate (L)</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Volumetric moisture content in unsaturated zone (L$^3$L$^{-3}$)</td>
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<tr>
<td>$\theta_0$</td>
<td>Initial volumetric moisture content in unsaturated zone (L$^3$L$^{-3}$)</td>
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<tr>
<td>$\theta_c$</td>
<td>Angle of inclination of between principle and global coordinate axis (-)</td>
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<td>$\theta_f$</td>
<td>Weighing coefficient (-)</td>
</tr>
<tr>
<td>$\theta_r$</td>
<td>Residual moisture content in unsaturated zone (L$^3$L$^{-3}$)</td>
</tr>
<tr>
<td>$\theta_s$</td>
<td>Saturation moisture content in unsaturated zone (L$^3$L$^{-3}$)</td>
</tr>
<tr>
<td>$\xi$</td>
<td>Local longitudinal coordinate (L)</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Radioactive decay constant for contaminant (T$^{-1}$)</td>
</tr>
<tr>
<td>$\rho_b$</td>
<td>Bulk density of the porous medium (ML$^{-3}$)</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Tortuosity of porous medium (-)</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>Global groundwater flow domain boundary (L)</td>
</tr>
<tr>
<td>$\Gamma_1$</td>
<td>Specified head boundary in groundwater flow model (L)</td>
</tr>
<tr>
<td>$\Gamma_2$</td>
<td>Specified flux boundary in groundwater flow model (L)</td>
</tr>
<tr>
<td>$\Gamma_3$</td>
<td>Head-dependent boundary in groundwater flow model (L)</td>
</tr>
<tr>
<td>$\nu_x$</td>
<td>Velocity of overland flow in the direction of channel flow (LT$^{-1}$)</td>
</tr>
<tr>
<td>$\psi_f$</td>
<td>Weighing coefficient (-)</td>
</tr>
</tbody>
</table>
\( \psi \): Pressure head in unsaturated zone (L)
\( \psi_0 \): Initial pressure head in unsaturated zone (L)
\( \Omega \): Global groundwater flow domain (L²)
\( \Omega_e \): Local groundwater flow domain (L²)

\( A \): Global coefficient matrix
\( B \): Global load vector
\( \hat{C}_g \): Global approximate vector for contaminant concentration in groundwater
\( f \): Vector of arbitrary functions
\( F \): Load vector
\( \hat{h}_g \): Global approximate vector for hydraulic head
\( J \): Jacobian matrix in Newton-Raphson scheme
\( M \): Mass matrix
\( n \): Unit normal vector to the boundary
\( S \): Stiffness matrix
\( x \): Vector of unknown variables

\( i, j, k, l, m, o \): Indices
Surface and Subsurface Flow and Contaminant Transport Modeling in Lower Altamaha Watershed

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Abstract

Large scale watershed modeling has long been an important challenge for the hydrologist. Numerous models have been developed to analyze possible flow patterns over a watershed in response to some precipitation event. Although most of these models used empirically-based lumped parameter formulations by neglecting or oversimplifying the underlying physical processes, they have served their purpose and provided basic data without going through a detailed analysis. In recent years, the trend has switched to a more fundamental understanding of the processes affecting the overall response of the watershed. In this regard, hydrologic modelers have directed their focus on physically-based distributed parameter models that are based on rigorous mathematical formulations of physics laws defining the flow of water over a watershed.

In this study, a hybrid surface/subsurface flow and transport model is developed that blends the powerful distributed parameter models with relatively simpler lumped parameter models. The proposed hybrid model solves the channel flow and saturated groundwater flow domains in continuous time using fully distributed physics-based formulations. This system is supported with the overland flow and unsaturated groundwater flow that uses lumped parameter descriptions in discrete time. This hybrid formulation decreases the computational requirements associated with overland and unsaturated zone domains in a large scale continuous watershed modeling task but still allows a representative description of the watershed flow processes.

In the proposed model, a one-dimensional channel flow model is dynamically coupled with a two-dimensional vertically-averaged groundwater flow model along the river bed. As an alternative to the commonly applied iterative solution technique, a so-called simultaneous solution procedure is developed to provide a better understanding to the coupled flow problem. This new methodology is based on the principle of solving the two flow domains within a single matrix structure in a simultaneous manner. The method eliminates the iterative scheme that is otherwise required to obtain the convergence of the solution and provides a faster solution.
In addition to the flow model, a coupled contaminant transport model is also developed to simulate the migration of contaminants between surface and subsurface domains. Based on its flow counterpart, the contaminant transport model dynamically couples a one-dimensional channel transport model with a two-dimensional vertically-averaged groundwater transport model. The coupling is performed at the river bed interface via advective and dispersive transport mechanisms. A modified extension of the proposed simultaneous solution procedure is also implemented to solve the coupled contaminant transport problem. The dynamic coupling provides the much needed understanding for the continuity of contaminants in strongly interacting surface/subsurface systems such as a river and an unconfined aquifer.

The coupled flow and transport models are finally applied to the lower Altamaha watershed in southern Georgia. The flow model is used to perform simulations of hydrologic and hydraulic conditions along the river and in the dynamically linked surfacial aquifer. The model predicted the flood patterns including the magnitude of peaks and their arrival times with sufficient accuracy. Under the given flow conditions, the transport model is then implemented to test alternative contaminant transport patterns both in the river and within the aquifer.

1. Introduction

1.1. General

Since the early days of watershed modeling, hydrologists have separated and isolated the hydrology of the system into its subcomponents. They have implemented discrete models for various hydrologic processes in an effort to simulate the response of the watershed to a hydrologic disturbance. Such models have been studied and improved constantly for decades and have currently evolved to a certain level of advancement. Today, many commercialized software are available to accurately simulate discrete flow and transport patterns in surface and subsurface flow pathways including rivers and aquifers.

It was perhaps in the early 1970s that hydrologic modelers have realized the fact that separating an otherwise strongly linked system would involve major errors in proper representation of the response characteristics. In this regard, the work of Freeze (1972a, 1972b) has been a milestone in the hydrologic simulation of watershed processes within the context of a ‘single’ entity. Surface and subsurface processes have thus begun to be modeled as parts of a complete system. It was not surprising to see that this development in hydrologic modeling has coincided with an era when computers and computing power has started to become easily accessible to hydrologic modelers. Consequently, modelers have, slowly but surely, started to develop coupled models within the last two decades. This effort is still on-going and facing some though challenges despite all computational advances achieved.
1.2. **Integrated Watershed Modeling**

The concept of integrated watershed modeling has emerged as a new understanding for the interactions between the surface and subsurface pathways of water. It defines the bi-directional linkage that implies the main rationale for the unity of the two systems. In this regard, surface flow processes such as channel and overland flow are integrated to subsurface flow processes in the unsaturated and saturated groundwater flow zones via the dynamic interactions at the ground surface and channel bed. Only with this kind of an approach, one can successfully quantify the volumetric and mass flux balances between the domains.

The highly dynamic interactions between overland flow and unsaturated zone flow determine the amount of infiltrating/exfiltrating flux at the ground surface. Similar interactions also occur at the river bed where channel flow seeps into the underlying unconfined aquifer or vice versa. Both of these interactions are regarded as important links between the components of the hydrologic cycle and are responsible in maintaining the continuity of the entire cycle. While these interactions may operate as safety barriers to extreme conditions by decreasing the intensity and severity of major hydrological events such as floods and droughts, it is also likely that the opposite scenario is true and they tend to amplify the strength of such events and cause significant loss of life and property. Therefore, it is of utmost importance to analyze these interactions systematically and develop management scenarios based on such quantitative assessments.

Modeling watershed processes in an integrated fashion is thus the ultimate goal of a state-of-the-art analysis. Although there is no doubt about the necessity of integrated watershed modeling, this process is a fairly complicated task even with the level of technological developments accomplished. Therefore, despite the advances in computational speed and capacity, integrated watershed models still require extensive computational times for large scale applications which in turn requires for the modeler to have a clear understanding of the temporal and spatial scales of the processes.

1.3. **Temporal and Spatial Scales of Watershed Processes**

Different flow pathways of the watershed experience entirely different time and space scales. These differences have a direct impact on the numerical discretizations of these sub-processes. One of the most evident of these differences is the time scale dissimilarities between the overland flow process and saturated groundwater flow process. While the former is a much faster pathway requiring time steps in the order of seconds, the latter is a fairly slow process and calls for much larger time steps in the order of days or even months. Such differences beyond doubt create problems in the numerical solution procedures. Moreover, these problems are even more pronounced when these two sub-systems are solved in an integrated fashion. Similar points of concern await the modeler in the spatial discretization of various domains as well. A perfect example of a space scale problem is experienced in the unsaturated zone. Space scale requirements of the unsaturated zone
models are several orders of magnitude smaller than their saturated zone counterpart, which becomes a major concern in integrated modeling applications.

In addition to varying scales of subprocesses, the modeler also faces the critical issues of a representative time scale that is of importance to all watershed flow pathways. This directly leads to the problem of assigning a time frame for the overall analysis of the processes. For long term simulations (i.e., seasonal or annual simulations) that most modelers would prefer, the existence of some of the more dynamic subprocesses becomes an issue. An example of such a condition is the overland flow process that only exists during a very limited time frame when compared to the other pathways of flow. Additional problems are present in the simulation of overland flow when one considers the boundedness of the process in spatial and temporal dimensions. It is not easy to identify well-defined temporal and spatial extents of the overland flow pathway and hence, a long term simulation of a large scale watershed clearly faces numerical difficulties when overland flow process is to be included in the analysis.

1.4. Research Needs and Objectives of the Study

Currently, the integration of watershed processes are implemented at limited spatial and temporal scales. Many integrated models are developed at the test bed scale to analyze the general consequences of the interactions between flow pathways. Only a limited number of such models are found to be applied at small experimental watersheds. In this regard, there is an emerging need to develop models which can be applied to large scale watersheds using real time data. Furthermore, the coupling mechanisms of the sub-processes also provide an open field for development where the current methodologies are based on discrete solution of surface and subsurface flow systems. In discrete solution procedures, linkage between the domains is achieved by (i) simplistic non-iterative methods in which results from the solution of one domain is directly fed into the other domain and does not accept any feedback from the solution of other domain, or (ii) iterative methods where solutions from one domain is fed to the other in a cyclic manner until sufficient convergence is achieved between two consecutive solutions. Currently, iterative techniques are regarded as the state-of-the-art for coupling surface and subsurface flow processes. However, it is also believed that there is room for progress in the sophistication of the coupling procedures such as the advanced simultaneous solution of both processes as proposed in this study.

Finally, despite the efforts to couple flow processes, hydrological modelers were hesitant in coupling contaminant transport processes. There is literally no model available that does perform a coupled surface-subsurface contaminant transport modeling at a watershed scale. Although this may be partially attributed to the current premature state of flow coupling, it clearly does not justify the lack of attention by the hydrologic modeler. It is believed that at least some of the efforts spent on flow coupling could be re-routed towards analyzing the relationships between surface and subsurface processes in terms of transport of contaminants.
Based on these facts, this study attempts to develop models that are directly applicable to large scale watershed systems. Coupled models of surface and subsurface flow processes are developed in an effort to provide a better understanding for the relative significance of the pathways that drive the hydrological cycle. Considering the numerical difficulties associated with mathematical representation and numerical solution of some of the flow processes, a hybrid modeling approach is proposed in this study. This approach offers the much needed relief that fully physically-based distributed models suffer from by compromising the process description of the problematic processes and proposing relatively simple empirical approaches in their representation.

Sophisticated coupling mechanisms are also studied in detail and a new, more efficient coupling mechanism is proposed and applied to large scale systems. This new simultaneous coupling technique attempts to solve surface and subsurface flow and transport processes simultaneously rather than implementing a sequential solution and an iterative improvement of the common parameters. In this regard, it is believed that this new methodology has a very wide open prospect for coupled hydrological modeling. In addition, this study also puts forward one of the possibly earliest applications of coupled contaminant transport modeling in large watersheds. The proposed approach uses a semi-simultaneous coupling of surface and subsurface transport mechanism and provides linkage via not only the generally used advective transport mechanism but also the commonly neglected dispersive transport mechanism as well.

1.5. Organization of the Report

With the above mentioned objectives, this report is organized in 6 main chapters and 1 appendix. In Chapter 2, a detailed literature review is done in which a thorough description of watershed models as well as watershed flow and transport processes are discussed. A summary of available coupling techniques and scale issues are also given in this chapter. The mathematical models of key watershed processes are discussed in Chapter 3 where the governing equations, initial and boundary conditions and the implemented numerical solution procedures of each process are presented from the perspective of large scale watershed modeling. Two coupled models are studied in detail and a hybrid modeling approach is proposed. The details associated with the new simultaneous coupling procedure are also presented in this chapter. In Chapter 4, the focus switches to the major transport processes and a coupled surface-subsurface contaminant transport model is presented. The governing equations, initial and boundary conditions and the numerical solution procedures of the proposed transport model is presented in this chapter of the report. The new coupled models of flow and transport are then used to simulate the hydrological and hydrochemical characteristics of the lower Altamaha watershed. The details of this application are given in Chapter 5. Finally, a conclusion and recommendations section wrap up the report in Chapter 6.
2. Background and Literature Review

In this chapter, background information on watershed processes and modeling principles are reviewed with special emphasis on different hydrologic processes encountered in a watershed. The mathematical description of these processes and their numerical solution are reviewed along with a discussion of alternative coupling mechanisms utilized to link various pathways in a watershed. After coupling processes are introduced, a detailed analysis of scale problems in watersheds is presented including the spatial and temporal scales that are common to various pathways. The chapter concludes with a discussion of the data requirements of watershed models.

2.1. Characteristics of Watershed Models

Models that describe watershed hydrology are classified according to several criteria. One of the most significant of these classifications is based on the spatial variability of the parameters that define the flow processes (Abbott and Refsgaard, 1996). In this regard, a distributed parameter model takes into account the spatial variability in all parameters of concern, whereas a lumped parameter model assumes the watershed to be single unit with variables and parameters representing average values for the entire catchment. From this perspective, a lumped parameter model downscales and simplifies a complex system to a single unit entity.

Another closely related classification of watershed models is based on system characteristics. Such a classification distinguishes models that are based on fundamental laws of physics from models that are solely based on certain empirical rules of input/output functions. In this regard, the so-called physically-based model describes the natural system using fundamental physics laws that define the movement of mass, momentum and energy by using complex mathematical representations (Abbott and Refsgaard, 1996). These mathematical relations are partial differential equations, integral-differential equations or integral equations including but not limited to the Saint Venant equations for channel and overland flow, Richards’ equation for unsaturated zone flow and Boussinesq’s equation for saturated groundwater flow. Such models are also known as ‘white box’ models expressing the fact that the details associated with the underlying processes are all known and clear to the modeler. Physically based models always display the characteristics of distributed models as they involve at least one spatial dimension and variations along this dimension. Well known examples of physically-based distributed models include the SHE model of Abbott et al. (1986a and 1986b), IHDM model of Beven et al. (1987), THALES model of Grayson et al. (1992) and MIKE SHE model of Refsgaard and Storm (1995).

On the opposite extreme, empirical models are developed with little or no consideration to the underlying physical theory and attempt to explain the natural behavior by using simple input-output relationships. In this regard, this type of a model is generally called a “black box” model about which the modeler has often little or no physical understanding of its processes. It serves as a simple mechanism that converts the input information to some sort
of an output response without any consideration of the internal characteristics of the process. Abbott and Refsgaard (1996) have further classified black box models into three main groups: (i) empirical hydrological methods; (ii) statistically-based methods; and, (iii) hydroinformatics-based methods. The empirical hydrological methods are amongst the best known black box models. Unit hydrograph theory and Soil Conservation Service (SCS) curve number method are examples of this type of model. The statistically-based methods include many models developed using regression and correlation analysis of the available data. These methods are also called the transfer function models that convert an input time series to some output time series. An example of this type of black box model is the antecedent precipitation index (API) model that correlates rainfall volume and duration, past days of rainfall and season of year to runoff. Finally, a new group of black box models called the hydroinformatics-based methods are developed in parallel with the recent advances in information technology such as artificial neural networks and genetic algorithms. It is, however, important to note that, regardless of the level of advancement achieved with an empirical model, it will always be one step behind the physics-based models as the latter provides a thorough and more correct description of the hydrological processes in a watershed. Furthermore, physics-based models also provide a suitable platform where all information associated with the watershed could be extracted without much difficulty.

Despite their drawbacks, however, empirically-based models are still extensively used due to the simplicity and speed of the analysis. Examples of empirically-based distributed parameter models include the ones that are developed to perform simple rainfall-runoff analysis such as the SCS curve number method (Still and Shih, 1985) or the ones that are formulated to carry out fairly complicated watershed analysis such as the Hydrologic Simulation Program-Fortran (HSPF) model (Donigian et al., 1995).

Another possible classification for hydrological models is carried out based on the time scale of the process. From a broader perspective, models could be continuous in time performing real time simulations or they could be discrete in time implementing simulations that are based on daily, monthly or even yearly-averaged values of model parameters (Singh, 1995). Nevertheless, this classification does not have clear-cut boundaries similar to the previously mentioned classifications due to the fact that even a continuous-in-time model uses certain time steps that, in essence, represent the average values within that time step. In this regard, one can argue that there would never be a continuous time model since the definition of the time step violates the continuity of the process. This discussion could further branch out when one realizes the fact that some of the watershed processes such as overland flow are so limited in time, when compared to others such as channel or groundwater flow, that continuous simulation of all watershed flow pathways in a simultaneous manner is simply not feasible with our current level of understanding. It is probably this motivation that forces the modelers to develop event-based models that run only during the time period when all watershed processes physically exist.
2.2. Hydrologic Flow Processes and Pathways in a Watershed

The hydrology of a watershed could be analyzed in two broad categories: (i) surface flow processes; and, (ii) subsurface flow processes. A combination of these two major flow categories defines the overall response of the system to a hydrologic input. The surface flow processes are further classified into channel and overland flow sub-systems where the surface flow depth, velocity and width clearly proposes the presence of two distinct domains which may or may not be analyzed separately depending on the purpose of the analysis. The channel flow is usually defined as the bulk movement of water in domains with relatively well-defined boundaries. It is considered to be the major conveyance medium in terms of the quantity of water transported downstream. The channel flow is characterized by high flow velocities and depths and is considered to be a fully-turbulent flow phenomenon (Chow, 1959). The overland flow subsystem, on the other hand, is defined over the entire surface area of the watershed with no well-defined boundaries. Although the small flow depths and velocities of overland flow suggest that the flow is in the laminar range, additional factors including rainfall impact, vegetation, channelized flow and the non-fixed bed phenomena complicates the problem. In this regard, a general consensus has been achieved among hydraulics experts that the overland flow covers both laminar and turbulent flows (Moore and Foster, 1990). Since overland flow occurs as an outcome of space and time variable precipitation input, it is represented by highly variable spatial distribution and temporal coverage. This major difficulty associated with overland flow becomes even more pronounced in the presence of small water depths and velocities and complicates accurate simulation of overland flow processes.

The subsurface flow is generally defined by the variably-saturated flow phenomena according to the level of saturation of the porous medium (Bear, 1979). The domain could be spatially and temporally variably-saturated depending on the overall flow behavior, boundary conditions and forcing functions. In general, the variably-saturated three-dimensional domain is subdivided into: (i) a saturated flow zone; and, (ii) an unsaturated flow zone according to the level of saturation of the porous medium. These two sub-systems are separated from each other by the groundwater table, below which, a saturated groundwater flow zone develops and above which, an unsaturated groundwater flow zone occurs. As the position of water table is spatially and temporally variable in a watershed, the domain that is considered to be saturated varies accordingly and any modeling effort must consider the associated consequences. Although the subsurface flow processes can be modeled as a single variably-saturated medium, it is generally treated as two separated systems linked to each other at the groundwater table. This artificial separation of variably-saturated subsurface flow phenomenon into saturated and unsaturated zones simplifies the analysis and provides a more straightforward understanding of the overall hydrologic conditions of the watershed.

In the light of the above discussion, the major watershed processes of concern are considered to be: (i) the channel flow; (ii) the overland flow; (iii) the unsaturated zone groundwater flow; and, (iv) the saturated zone groundwater flow. The mathematical and
physical characteristics as well as possible numerical solution methodologies of these watershed flow pathways are discussed in the following sections.

2.2.1. Channel Flow

The channel flow is characterized with small water depths when compared to other major systems such as seas, oceans and large inland lakes. While these large flow processes are described by the general three-dimensional hydrodynamic equations of fluid flow (i.e., the mass conservation equation and the Navier-Stokes equations of motion), many flows systems of interest to the hydrologic modeler including channel flow are characterized by small flow depths in the vertical dimension compared to their lateral and longitudinal flow dimensions. For such systems, the two-dimensional depth-averaged hydrodynamic equations are generally deemed sufficient to describe this shallow water flow phenomenon as it occurs in rivers, estuaries, shallow lakes and over land surfaces. The shallow water equations that are used to model these flows are developed by vertically averaging the general three-dimensional equations of mass continuity and momentum (Dronkers, 1964; Chow and Ben-Zvi, 1973; Zhang and Cundy, 1989; Weiyan, 1992).

The channel flow is a good example of shallow water flow system. It has a significantly small vertical flow component when compared to its longitudinal and transverse flow dimensions. Furthermore, channel flow in small to moderate sized rivers is also characterized by small widths such that velocity and depth are assumed to vary only in the direction of flow and a single velocity and depth is assumed to govern the entire channel width. Under these assumptions, river channel flow is described by the one-dimensional analog of the three-dimensional hydrodynamics equations and is generally known as the Saint-Venant equations after French hydraulic engineer B. de Saint-Venant who has introduced them in late 19th century (Strelkoff, 1969).

The assumption of one-dimensional flow has been widely accepted and numerous models have been developed for analyzing unsteady non-uniform flow in open channels (Liggett and Woolhiser, 1967; Baltzer and Lai, 1968; Strelkoff, 1970; Fread, 1993; Havno et al, 1995). Particularly for large scale applications such as watershed modeling, one-dimensional flow assumption is the only practically available option to the hydrologic modeler (Refsgaard and Storm, 1995; Jha et al., 2000).

Even though the Saint-Venant equations form the basis of the general mathematical model of the unsteady non-uniform flow in channels, they should be modified for application to natural waterways since natural systems such as rivers and streams show significant variability from man-made channels in terms of channel geometry, channel bed roughness and river form. These characteristics are extremely important for alluvial systems where braiding and meandering are commonly observed. As a result, a number of researchers including Fread (1976) and DeLong (1986 and 1989) have modified the Saint-Venant equations so that they could be applied in river channels. They have introduced the effects of complex channel geometry (i.e., channel-floodplain system) and meandering pattern in the equations. Upon these modifications, the Saint-Venant equations became capable of
accounting for the effects of the floodplain, inactive (off-channel or dead) storage and the meandering ratio (sinuosity factor) of the river.

Both the original and the modified Saint-Venant equations have various simplified forms, which are obtained by neglecting some of the terms in the one-dimensional conservation of momentum equation. These simplified forms of the momentum equation coupled with the continuity equation yield a number of approximate distributed flow methods. Without any simplification, the full Saint-Venant equation is also known as the dynamic wave model. It is the only model that can accurately simulate the backwater effects in channel by allowing the propagation of the changes in discharge and water depth in the upstream direction. The local and convective acceleration terms as well as the pressure force term describe this upstream movement of changes in flow momentum. The dynamic wave model is the model of choice when the backwater effects are significant or the channel slope is mild (Sturm, 2001). If the local and convective acceleration terms in the momentum equation are neglected, the so-called diffusion wave model is obtained. Diffusion wave model can also be used to simulate the backwater effects only to a certain degree via the pressure force term. Therefore, it cannot be the model of choice when significant backwater effects are present. The diffusion wave model is further simplified by neglecting the pressure force term to obtain the simple kinematic wave model that is known to be the simplest channel flow model. The kinematic wave model assumes that friction slope is equal to channel bed slope and does not allow the simulation of backwater effects as flood wave can only travel downstream (Sturm, 2001).

The complete Saint-Venant equations are a set of partial differential equations with two independent and two dependent variables. There is no analytical solution to these equations except in a few special cases. In general, the only choice of solution for these equations is through the application of numerical techniques, which are classified as: (i) method of characteristics; (ii) finite difference methods; and, (iii) finite element methods. These methods can be further classified as explicit or implicit methods depending on the solution approach selected.

Among the available three solution procedures, the method of finite elements is seldom used to solve Saint-Venant equations of unsteady flow (Cooley and Moin, 1976; Szymkiewicz, 1991; Blandford and Ormsbee, 1993; Szymkiewicz, 1995). This is mainly due to the fact that the finite element method does not offer any advantages over the method of characteristics or the finite difference technique in a one-dimensional setup. The power of finite element method becomes apparent in two- or three-dimensional treatment of unsteady flow routing in natural waterways, such as very wide river systems and estuaries.

The method of characteristics was the first successfully applied technique for the solution of Saint-Venant equations. The application of this technique required a transformation of the original partial differential equations to their characteristic forms, which are ordinary differential equations. In the 1960's, Liggett and Woolhiser (1967) and Streeter and Wylie (1967) developed explicit solution techniques to the characteristic forms of the Saint-
Venant equations. Similarly, Amein (1966) and Wylie (1970) worked out some implicit solution methods for the same characteristic forms of the original equations. The characteristic method is applied either on a characteristic (curvilinear) grid or a rectangular grid in the $x$-$t$ solution plane. The former is not suitable for application in natural waterways with irregular geometry (Fread, 1985). The latter, also known as the Hartree method, requires the interpolation formulae meshed within the finite difference solution procedure. This restriction has limited the application of the method of characteristics to flood routing (Fread, 1985). However, it is still used in explicit and implicit finite difference techniques for a more accurate approximation of boundary conditions (Sturm, 2001).

The finite difference methods are based on the principle of transforming the governing differential equations into algebraic equations by approximating the derivatives in terms of difference equations. In explicit finite difference methods, the solution of Saint-Venant equations advances point by point along one time line in the $x$-$t$ solution domain until all the unknowns associated with that time line have been evaluated. Then, the solution advances to the next time line. The numerical solution of the explicit method is quite straightforward and it is easily programmed. In implicit methods, the solution of the Saint-Venant equations advances from one time line to the next simultaneously for all points along the time line. Hence, the implicit method is numerically more complex and difficult to program. The major difference between the explicit and the implicit methods is the number of unknowns used from the time line where the solution is searched. In the explicit scheme, only the approximations of the time derivative involve the unknown variables, whereas in an implicit scheme, the approximations of all derivatives (i.e., time derivative, space derivative and non-derivative terms) contain the unknown variables and are solved simultaneously (Fread, 1985).

The development of explicit techniques began with the pioneering work of Stoker (1953) and followed by Liggett and Woolhiser (1967) and Strelkoff (1970). Even though the explicit scheme is relatively simple compared to the implicit scheme, it has serious restrictions in the size of the computational time step in order to achieve numerical stability. It was this motivation that led to the development of implicit schemes, which was originally formulated by Preissmann (1961). Following his work, Amein and Fang (1970), Chaudhry and Contractor (1973), Amein and Chu (1975) and Fread (1976) have also developed implicit schemes to solve flood routing problems. The implicit method of Preissmann (1961) later became the method of choice for channel flow analysis due to its flexibility in using large time steps with unconditional stability and is implemented in many studies after 1970s.

2.2.2. Overland Flow

The overland flow is another example of shallow water flow that can be analyzed with vertically-averaged equations. It is considered to be an important subprocess of watershed hydrology. Regardless of its source (i.e., infiltration excess or saturation excess), it is considered to be the major contributor of channel flow. However, unlike channel flow, it is characterized by even smaller water depths that are in the order of a less than a couple of
centimeters which makes its analysis more difficult when compared to channel flow. Although small depths and velocities propose a laminar treatment of the process, other parameters such as the rainfall impact, highly variable roughness patterns and channelization favor a turbulent analysis for the process. It is because of these complications the overland flow is generally assumed to experience all possible aspects of flow hydraulics in a time and space dependent fashion. In the context of a general watershed model, however, such complications are generally included in to one roughness parameter and the entire overland flow phenomena is modeled as a turbulent flow similar to its channel flow counterpart. While this assumption may not be true at all times, it is the only feasible way to tackle the associated difficulties.

Another major characteristic of the overland flow is its temporarily discontinuous flow behavior. Unlike any other watershed flow processes, the overland flow is highly driven by external sources that are intermittent in time. While channel flow and groundwater flow are generally considered to be continuous flow processes, overland flow shows discontinuities in time and space as a direct consequence of the temporally and spatially non-uniform source/sink function. In this regard, overland flow does not have well-defined flow boundaries. It may be regarded as the only flow process that experiences a continuously changing flow domain, which is one of the reasons for the difficulties encountered in its numerical simulation.


Similar to the channel flow case, both the complete and the simplified forms of the two-dimensional Saint-Venant equations of overland flow are extensively used. Chow and Zvi (1973), Katopodes and Strelkoff (1979), Akanbi and Katopodes (1988), Zhang and Cundy (1989), Tayfur et al. (1993), Playan et al. (1994), Zhao et al. (1994), Hong and Mostaghimi (1997), Fiedler and Ramirez (2000) and Esteves et al. (2000) have preferred the full dynamic wave approach. However, their studies were all conducted on a limited spatial extent including laboratory experiments or test bed hypothetical runs. None of these studies were actually done at a realistic watershed scale. On the other hand, all overland flow models that are applied at the watershed scale used either the non-inertia wave or kinematic wave assumptions. These simplifications essentially made the process more suitable for

In general, two-dimensional overland flow could only be solved using numerical methods. Among the available three solution procedures, the method of characteristics is rarely applied due to the difficulties encountered in multi-dimensional characteristics methods. Except for the model of Katopodes and Strelkoff (1988), there is no bi-directional method of characteristic application of overland flow. On the other hand, both the finite element and the finite difference techniques have been widely used and became the method of choice for two-dimensional overland flow modeling. While the works of Chow and Zvi (1973), Hromadka and Lai (1985), Hromadka and Yen (1986), Zhang and Cundy (1989), James and Kim (1990), Tayfur et al. (1993), Playan et al. (1994), Julien et al. (1995), Feng and Molz (1997), Esteves et al. (2000), Friedler and Ramirez (2000), Chang et al. (2000) and Dutta et al. (2000) have all used explicit and implicit finite difference methods; Akanbi and Katopodes (1988), Marcus and Julien (1990), Zhao et al. (1994), Hong and Mostaghimi (1997), Gottardi and Venutelli (1997) have preferred finite element technique. Moreover, Di Giammarco et al. (1996), Gottardi and Venutelli (1997), Lal (1998) have used mass conservative control volume finite element method. As seen from the wide variety of studies, there is no direct preference for a particular method. However, finite element method has obvious advantages over finite difference method to discretize domains without any particular shape and size such as a watershed.

2.2.3. Unsaturated Zone Flow

The movement of moisture in the variably saturated flow is often modeled by using the Richards’ equation and closed by constitutive relations to describe the relationship among fluid pressures, saturations and hydraulic conductivities. When the groundwater flow is studied in two zones separated by the water table, the region of low saturation values between the ground surface and the water table is often called the unsaturated zone to distinguish it from its saturated counterpart that is found below the water table. The unsaturated zone is characterized by spatially and temporarily varying levels of below saturation water contents and associated capillary pressure heads. A major characteristic of flow in the unsaturated zone is the dependency of the hydraulic conductivity of the medium to the level of saturation which generally becomes a strong non-linear function for many soil types. Therefore, in addition to the complexity of governing Richards’ equation, the complexity of constitutive relationships that link the level of saturation to capillary pressure and hydraulic conductivity further complicates the governing equations and its numerical solution.

Although the unsaturated zone flow is three-dimensional in principle, it is often approximated with its one-dimensional counterpart along the vertical domain. This simplification essentially treats the unsaturated zone as a vertical link between the surface
and the water table. As long as the source of moisture in this zone is either the infiltrating flux or rising water table, this simplification works fairly well. Particularly, in low land areas with mild surface topography, one can consider the unsaturated zone as columns of soil providing a conduit for bidirectional movement of soil moisture. Such an approach is widely used in large-scale watershed modeling including the SHE model of Abbott et al. (1986). A three-dimensional variably-saturated flow is practically not possible to implement in terms of computational resource limitations in large scale watershed models. Furthermore, Singh and Bhallamudi (1998) has found out that the results don’t show significant differences when the unsaturated zone is modeled as one-dimensional (i.e., vertical) as opposed to a possible two-dimensional (i.e., vertical-horizontal) treatment.

While Richards’ equation is originally based on the capillary pressure as the dependent variable, numerous researchers have developed various modified forms by changing the dependent variable of the equation. Over the years, three different forms of the Richards’ equation has been found to be widely applied by the soil scientist: (i) the pressure head-based equation; (ii) moisture content-based equation; and, (iii) mixed form of the equation with both the pressure head and the water content explicitly appearing as dependent variables of the equation.

The original pressure head based equation is applicable to all levels of saturation in the porous medium. It performs in a superior way under saturated conditions when some of the other forms fail to properly represent the flow conditions (Huang et al., 1996). This behavior is mostly related to the fact that the pressure head is a continuous function both in saturated and unsaturated medium under non-homogeneous soil profiles. Unfortunately, the pressure head-based equation does not perform as good as the water content-based equation under significantly dry conditions (Huang et al., 1996). Especially under the condition of infiltration to a very dry soil, the pressure based form develops large mass balance errors due to the highly nonlinear nature of specific moisture capacity and notably underestimates the infiltration depth. Regardless of the limitations associated with it, this original form of the equation has been used extensively in solving both the unsaturated zone and variably saturated-unsaturated zone flow problems (Neuman, 1973; Narasimhan et al., 1978; van Genuchten, 1982; Milly, 1985; Feddes et al., 1988; Celia et al., 1990; Paniconi et al., 1991; Gottardi and Venutelli, 1993a; Rathfelder and Abriola, 1994; Pan and Wierenga, 1995; Pan et al., 1996; Romano et al., 1998; Williams et al., 2000; van Dam and Feddes, 2000).

To alleviate the problems associated with the pressure head-based form of the governing equation, a moisture-content based form was proposed as an alternative formulation of the unsaturated zone flow. This formulation is found to be superior in terms of mass conservation, particularly in the discrete approximations of its numerical solution such as finite element and finite difference methods (Hills et al., 1989; Gottardi and Venutelli, 1993a; Pan and Wierenga, 1997). Moreover, the hydraulic functions are less nonlinear when expressed in terms of moisture content rather than capillary head, particularly when modeling infiltration into a relatively dry medium (Williams et al., 2000). However, the water content-based form of the equation was also limited in application to variably saturated-unsaturated flow since it was not able to properly simulate the saturated
conditions. When the flow domain gets locally or completely saturated, the equation degenerates since the time rate of change of the moisture content becomes zero (Celia et al., 1990). In addition, using moisture content as the dependent variable introduces problems of continuity in the domain since it is not a state variable which is always continuous in space regardless of the soil inhomogeneities.

To overcome the difficulties associated with both the pressure-based and the moisture content-based forms of the Richards equation, a so-called mixed-form has been proposed, which uses both the moisture content and the pressure head as the dependent variables. The mixed form has both the superior mass conservation characteristics of the moisture content-based equation as well as the unlimited applicability to both saturated and unsaturated regions of flow that the pressure-based equation offers (Celia et al., 1990). In this regard, the numerical solution of the mixed form found wide applicability in the last decade and many researchers used this form to model the flow in variably saturated-unsaturated media (Celia et al., 1990; Gottardi and Venutelli, 1993a; Hong et al., 1994; Huang, et al., 1996; Tocci et al., 1997; Miller et al., 1998; Williams and Miller, 1999; Zhang and Ewen, 2000; de Vasconcellos and Amorim, 2001; Zhang et al, 2002).

Apart from these standard forms of the equations, some researchers did not directly use these three forms of the governing equation but rather applied certain transformation functions to smoothen the strong non-linearity of the constitutive functions (Pan and Wierenga, 1995; Pan et al., 1996; Pan and Wierenga, 1997; Williams and Miller, 1999; Williams et al., 2000). Event though these transformation techniques provide some relief to the problems associated with the numerical solution, they did not find wide applicability mainly due to the fact that they are only an approximation to the original equation and lack any underlying physical theory.

Regardless of the form of Richards’ equation used, one needs to supplement the governing equation with the auxiliary equations to complete the mathematical representation of moisture movement in the unsaturated zone. These auxiliary relations are the soil-water retention and hydraulic conductivity relationships that correlates the capillary pressure head to soil moisture and hydraulic conductivity (Bear, 1979). Although these relations are known to yield solutions to the Richards equation, it is rarely available in the extent that a distributed watershed model would require in terms of spatial variability. Therefore, researchers developed numerous empirical formulae to provide the relation between capillary pressure head and soil moisture as well as capillary pressure head and hydraulic conductivity. The most commonly used ones of these relations are the ones proposed by Brooks and Corey (1964), Campbell (1974), Mualem (1976), Clapp and Hornberger (1978) and van Genuchten (1980). It is important to note that the original forms of these relations did not consider the phenomenon of hysteresis and pressure head is considered to be a single-valued function of moisture content.

The extreme variability and complexity of geological materials, dry initial conditions, varying boundary conditions and the strong non-linearity between the pressure head and moisture content as well as the pressure head and hydraulic conductivity make the solution
of Richards’ equation quite a challenge, particularly within acceptable limits of accuracy
and computational effort. Since analytical solutions are only possible when these nonlinear
relationships are linearized and simplified (Tracy, 1995), numerical techniques are the only
available method for the solution. In numerical solution of the Richards’ equation, the
spatial discretization is commonly performed by: (i) finite difference; and, (ii) finite
element methods (van Genuchten, 1982; Milly, 1985; Celia et al., 1990; Hong et al., 1994;
Rathfelder and Abriola, 1994; Pan and Wierenga, 1995; Pan et al., 1996; Huang et al.,
1996; Miller et al., 1998; van Dam and Feddes, 2000; Zhang and Ewen, 2000; Zhang et al.,
2002). The standard temporal discretization technique used to approximate the Richards’
equation is the one-step Euler approach and the most common solution method uses a fully
implicit time approximation of the time derivative. Recently, variable step size variable
time order integration methods are also used to discretize the temporal derivatives (Tocci et
al., 1997; Miller et al., 1998; Williams and Miller, 1999).

2.2.4. Saturated Zone Flow

The saturated groundwater zone is defined as the domain below the water table. Since it is
bounded by a dynamically changing water table, this zone is also known as the unconfined
aquifer. The significance of this zone comes from the fact that it provides a link to other
watershed processes such as the unsaturated zone as well as the channel flow zone.
Therefore, it is a critically important part of the watershed hydrology. The saturated
groundwater flow is modeled by the Boussinesq’s equation that describes the movement of
flow in porous medium. Darcy’s law is the momentum equation embedded in the mass
conservation equation (Bear, 1979).

The saturated zone flow could either be characterized by a three-dimensional groundwater
flow model or a vertically-averaged two-dimensional groundwater flow model. Many
modelers have used a three-dimensional representation of the groundwater flow such as
Frind and Verge (1978), Huyakorn et al. (1986) and McDonald and Harbaugh (1998).
Others such as Aral (1990) have preferred vertically averaged two-dimensional
representation considering the essentially two-dimensional horizontal flow pattern of
groundwater in aquifer systems. It is, however, important to note that all of these models
are developed as multi-layer aquifer models and are certainly applicable to deep aquifer
systems. In the case of an unconfined aquifer, however, a three-dimensional representation
might be necessary when the aquifer is under influence of sources/sinks. In the close
vicinity of the wells, for example, flow becomes three dimensional. Vertically-averaged
models are only suitable when the change in water table is not significant compared to the
saturated aquifer thickness. Therefore, in cases where the assumption of vertical averaging
might be violated, these models should be applied with utmost caution.

The numerical solution of the saturated groundwater flow equation is performed by finite
element or finite difference methods. The finite element method has found a wide
application in the field of groundwater modeling and numerous models used the finite
element discretization (Huyakorn et al., 1986; Aral, 1990). The finite difference method is
also applied commonly and the well known groundwater flow model MODFLOW used this
discretization (McDonald and Harbaugh, 1998). Today, the saturated groundwater flow modeling has reached to a certain level of sophistication where several commercial software packages have been developed and used with success.

2.3. **Hydrologic Transport Processes and Pathways in a Watershed**

The contaminant transport phenomenon in a watershed is a strong function of the flow pathways and their characteristics. It is generally not possible to consider a transport problem without properly identifying the governing flow patterns. Therefore, exactly the same approach needs to be applied when the transport problem is confronted. In this regard, one could analyze the transport of contaminants in surface and subsurface domains and implement proper linkages between these two systems. These two subsystems could further be classified as was done in flow analysis. It is, therefore, logical to analyze the contaminant transport in watershed as channel and overland transport in the surface subsystem and saturated and unsaturated zone transport in the subsurface system.

2.3.1. **Channel Transport**

The contaminant transport in channels is the most studied aspect of the general mass transport process in a watershed. It is not only the fastest transport mechanism but also occurs in a medium that is of utmost concern to humans. Consequently, many models have been developed to simulate the migration of contaminants along the channel. In the majority of these studies, the focus of the attention was directed towards the general characteristics of the transport equation.

Contaminant transport in a channel is a three dimensional phenomena. Even with the assumption of instantaneous vertical mixing, the transport process continues to be a two dimensional event until complete mixing is achieved in the transverse direction. Only after this point, the transport process can be effectively modeled with a one-dimensional behavior (Fischer et al., 1979). Although this condition limits the applicability of many models, one-dimensional transport modeling has been the choice of many researchers in analyzing transport phenomenon in channels and rivers. However, the modeler should always be concerned and on alert about the capabilities and the limitations of the one dimensional approach for contaminant transport modeling in channels.

Even with the simplifying one-dimensional approximation approach, the numerical solution of the advection-dispersion equation is still a complicated numerical problem. Unfortunately, the advances achieved in the field of numerical modeling of partial differential equations do not lead to a globally accepted efficient algorithm to solve the advection-dispersion equation. Even though the equation looks simple, it mathematically shows a dual behavior in terms of its characteristics depending on the relative significance of various terms of the equation. For advection dominated flows, the equation shows the characteristics of a hyperbolic equation, whereas it becomes a parabolic partial differential equation when the dispersion is the dominant term (Holly and Preissmann, 1977; Leonard, 1979). Considering the fact that this changing behavior of transport phenomenon could
occur in a time- and space-dependent fashion, the numerical solution becomes an extremely challenging task. Therefore, any numerical method attempting to solve the equation is expected to satisfactorily represent and address these challenges.

Several numerical solution techniques are implemented to solve the advection dispersion equation. These methods can be classified as: (i) Eularian methods including the finite difference, finite element or finite volume methods; (ii) Lagrangian methods; and, (iii) Eularian-Lagrangian hybrid methods. As all major problems associated with the equation are linked to the advection operator, most of the literature is focused on handling the difficulties associated with the numerical solution of advection. Many researchers worked on finding more efficient algorithms to treat advection component of the equation since the remaining terms such as the dispersion and decay operators as well as the sink/source terms do not pose any additional difficulties in the numerical solution. While some researchers focused on low (i.e., first and second) order conventional Eularian techniques (Tucci and Chen, 1981; Bencala, 1983; Bencala and Walters, 1983; Leonard and Noye, 1989; Ristenpart and Wittenberg, 1991; Runkel and Chapra, 1993; Chen and Falconer, 1994; Jaque and Ball, 1994; Islam and Chaudhry, 1997; Wang and Lacroix, 1997; Geisdal and Teigland, 1998; Runkel, 1998, Zhang, 1998), some others preferred higher order conventional Eularian techniques (Hirsch, 1975; Adam, 1977; Basco, 1984; Komatsu et al., 1985, Falconer and Liu, 1988; Leonard and Noye, 1989; Noye, 1990; Stamou, 1991; Leonard, 1991; Stamou, 1992; Chen and Falconer, 1992; Chu and Fan, 1998; Chu and Fan, 1999; Radwan, 1999; Spotz and Carey, 2001) to solve the advection operator. Although a common ground for all Eularian methods is the fixed grid structure that these methods are based on and is the main reason why these methods are so popular for, higher order methods utilize more nodes than the standard low order methods in an effort to reduce the false smearing and false oscillation problems of such methods particularly around steep front regions at the expense of computational power (Leonard, 1979).

In another line of work, several researchers proposed using Lagrangian and Eularian-Lagrangian hybrid algorithms to treat the troublesome advection operator (Holly and Preissmann, 1977; Leonard, 1979; Glass and Rodi, 1982; Bedford et al., 1983; McBride and Rutherford, 1984; Jobson, 1987; Yu and Li, 1994; Oliveira and Baptista, 1995; Manson and Wallis, 1995; Manson and Wallis, 2000; Manson et al., 2001). Pure Lagrangian methods follow the natural motion of the water mass along a changing mesh, which makes them computationally cumbersome due to the necessity to keep track of moving coordinates. Hybrid techniques, on the other hand, combine the advantageous aspects of Eularian and Lagrangian methods. They solve the advection operator with the powerful Lagrangian based particle tracking algorithm over a fixed Eularian grid. Despite the increasing popularity of hybrid schemes, some major drawbacks are to be resolved before they can become a reliable contaminant transport method. One of the major limitations of such methods lies in the fact that Lagrangian treatment of flow still did not develop to become the method of choice mainly due to the difficulties involved in its coding and the lack of intuitive analysis capabilities that the Eularian methods provide. Finally, they are implemented and experimented with relatively simple flows and has not been put to tests on real channel systems involving network of channels. They are not currently used in well-
developed water quality models and the accurate algorithms are yet to be formulated for complex systems such as river networks before these models could be applied in large scale watershed modeling. Because of these difficulties, the fixed grid Eularian schemes are still commonly implemented and improved as the most popular solution technique. Particularly, higher order schemes are increasingly used in Eularian framework to increase the accuracy of these methods under extreme conditions such as flows involving sharp concentration gradients.

2.3.2. Overland Transport

Overland transport of contaminants is vital for quantifying land-based distributed pollution such as the release of nutrients, pesticides and other dissolved hazardous chemicals from agricultural fields into surface runoff. The soil chemical loss to overland flow is an extremely complex phenomenon that is dependent on various factors including but not limited to the chemical application rate, soil chemical kinetics, mass transport in soil matrix, mass transfer in overland flow and overland flow pattern (Wallach and Shabtai, 1992). Within watershed modeling framework, the analyst is mostly focused on determining the flow and mass transfer patterns of overland processes. From another perspective, the process becomes the concern of the watershed modeler after the contaminant is released from the soil.

The temporarily discontinuous behavior of overland flow over the land surfaces influences the transport of contaminants. The contaminant might be released and transported with the flow to a certain distance from its point of origin but then re-accumulate at this new point if overland flow is not persistent to reach to a channel and cease due to several loss mechanisms. This behavior further complicates the analysis of overland transport of contaminants.

Numerous models simulating overland transport characteristics are developed by various researchers including but not limited to Akan (1987), Yeh et al. (1998), Yan and Kahawita (2000), Garcia-Navarro et al. (2000) and Wallach et al. (2001). While the studies of Yeh et al. (1998) and Yan and Kahawita (2000) were based two dimensional analysis of overland transport, Garcia-Navarro et al. (2000) and Wallach et al. (2001) worked on more simplistic one-dimensional models. Garcia-Navarro et al. (2000) and Yan and Kahawita (2000) have used a dynamic wave approach to model the overland flow patterns whereas Yeh et al. (1998) preferred non-inertia wave approach and Wallach et al. (2001) used a simpler kinematic wave approximation. These researchers have also implemented a variety of numerical solution schemes. While Yeh et al. (1998) have used a Eularian-Lagrangian finite element method, Garcia-Navarro et al. (2000) implemented a Eularian-Lagrangian finite difference method. On the other hand, Yan and Kahawita (2000) and Wallach et al. (2001) implemented standard Eularian finite difference techniques to solve the transport equation. It is therefore clearly seen that no particular method is favorable compared to the other one. However, the general suitability of finite element methods to processes with irregular domains also applies to overland flow.
2.3.3. Unsaturated Zone Transport

Contaminant transport in the unsaturated zone plays an important role in many areas of agriculture and engineering. The analysis of the migration of fertilizers into the soil matrix and potentially becoming pollutants for the saturated groundwater system is one of these many areas. Therefore, a clear understanding of contaminant transport in the unsaturated zone, including proper quantification of the relevant transport processes is important for the engineer (van Genuchten, 1982). Although high dimensional modeling of the unsaturated zone transport is possible, the major pathway of concern is the vertical movement of contaminants which eventually reaches and pollutes the saturated groundwater reservoir. In this regard, the focus is kept on only the one dimensional unsaturated zone transport models.

The major transport mechanisms responsible for vertical migration of contaminants are again advection and dispersion. Hence, the one-dimensional transport equation has a very similar form to its counterpart in channel flow with the exception of the relative magnitudes of advection velocities and dispersion coefficients. Advection in unsaturated zone occurs in a much slower fashion and this assists the modeler in terms of the success of the numerical algorithm. In this regard, standard Eularian finite difference and finite element methods have generally been the method of choice in numerous models including HYDRUS (Simunek et al., 1998), TETRANS (Corwin and Waggoner, 1990) and VLEACH (Ravi and Johnson, 1993).

2.3.4. Saturated Zone Transport

The advection-dispersion equation describing the contaminant transport in saturated groundwater exhibits similar characteristics to its counterpart in channel. Although the advection operator is still the major area of concern, the severity of the problem is generally milder in groundwater transport due to the significantly slower advection velocities in aquifers. It is generally accepted that there is at least 4-5 orders of magnitude difference between the advection velocities in the channel and in the aquifer. This condition provides certain amount of immunity to the problems associated with the advection operator.

Similar to its flow counterpart, the contaminant transport in groundwater could be analyzed with either a three-dimensional model or a vertically-averaged two dimensional model. The decision follows the same criteria depicted in the flow model selection and a similar approach is to be implemented to simulate the transport phenomenon.

The transport modeling in groundwater flow is generally done with: (i) standard Eularian finite difference or finite element methods (Voss, 1984; Huyakorn et al., 1985; Faust et al., 1990; Simunek et al., 1998); (ii) Lagrangian methods (Bear and Verrujit, 1987; Tompson and Gelhar, 1990; LaBolle et al., 1996); and, (iii) mixed Eularian-Lagrangian hybrid methods combining Lagrangian treatment of advection with the standard finite element or finite difference schemes for non-advection terms (Neuman, 1984; Celia et al., 1990; Yeh, 1990; Bentley and Pinder, 1992; Zhang et al., 1993; Yeh et al., 1993; Binning and Celia,
1995; Oliveira and Baptista, 1995). In spite of all the advances achieved and new techniques developed, there is not a single technique that can yield completely satisfactory solutions to the numerical solution of advection-dominated contaminant transport and it remains to be a difficult problem due to the often contradictory needs to suppress numerical dispersion, avoid artificial oscillation and conserve mass.

2.4. Coupling of Flow Mechanisms

During the last thirty plus years of computerized modeling, many models have been developed to simulate the response of a watershed to an unsteady, non-uniform, spatially-variable precipitation event. Often, these models separated the watershed into surface and subsurface components and focused on only one of these hydrological processes. Although this artificial separation of an otherwise linked system helped to reduce most of the problems associated with physical process description as well as its numerical solution, it lacked to describe the system accurately and resulted in numerous discrete models of limited applicability. Therefore, an integration mechanism between surface and subsurface flows is particularly important for models of watershed hydrology where the response of the system is based on simultaneous interactions between these two major flow domains.

The analysis of the hydrologic cycle reveals the fact that surface and subsurface flow processes are linked at a number of interfaces. The most obvious one of these interfaces is the ground surface where overland flow and unsaturated zone flow are linked to each other via the infiltration/exfiltration flux. The direction of the interacting flux is not only dependent on the overland flow conditions but also a strong function of the level of saturation of soil moisture. The two overland flow initiation mechanisms (i.e., saturation from above and saturation from below) are strongly related to these interactions as well as other factors such as the topography, land cover/use and rate of precipitation. Another major interface linking surface and subsurface flow processes is the river channel bottom. The seepage flux is responsible for providing the linkage between the two systems. The direction of the flux is a function of the relative values of groundwater head and river water stage.

The mechanism that links surface and subsurface components at the ground surface is the interaction between soil water content and infiltration of water to the ground. In most of the surface flow models, infiltration is modeled as a sink for overland flow and approximated by semi-empirical infiltration formulae such as that of Green and Ampt (1911), Horton (1933) or Philip (1957). On the opposite end, most subsurface models take the infiltrated water as a source for groundwater flow. This separated modeling approach is often deemed sufficient for watersheds with relatively low permeability soils (Freeze, 1972b). In watersheds with high permeability soils, interaction between surface and subsurface flow components becomes important especially during overland flow initiation (Morita and Yen, 2002). It has been observed that the surface flow is overestimated during the rising part of the hydrograph and underestimated during the recession part when surface-subsurface interaction is neglected (Wallach et al., 1997). In this regard, it is important to couple
surface and subsurface components to obtain accurate and comprehensive watershed modeling (Morita and Yen, 2002).

Depending on the accuracy required and numerical and computational complexity allowed, there are numerous techniques to couple surface and subsurface flow components: (i) true simultaneous coupling; (ii) iterative (internal) coupling; (iii) non-iterative (external) coupling; and, (iv) sink function type coupling (i.e., also known as “no” coupling). Except for the sink function type coupling, all three methods are based on linking partial differential equations of surface and subsurface flow via infiltration and seepage as the internal boundary conditions. In sink function type coupling, however, infiltration is simulated with empirical equations, which are based on soil characteristics.

The true simultaneous coupling is the ultimate, most advanced method of interacting surface and subsurface flows. The technique is based on numerically solving the surface flow, subsurface flow and the common internal boundary condition between the two as a set of simultaneous equations at each time step. Since the equations are solved simultaneously, the result directly yields the unknown quantities. This type of coupling is extremely difficult and this study is believed to be one of the earliest examples of true simultaneous coupling of watershed processes. The works of Gunduz and Aral (2003a, 2003b) are early examples of models implementing this technique. The true simultaneous coupling of watershed flow processes is deemed to be very promising and there is a wide open field for further research. Particularly, with the ever increasing computational power of personal computers, watershed models based on true simultaneous coupling is expected to emerge in the near future.

In iterative (internal) coupling, the equations of surface and subsurface flows are solved separately but iteratively at each time step of the solution. The link between the two is supplied by the infiltration equation represented as a gradient-type expression. The technique provides fairly accurate solutions at the expense of computational cost. Furthermore, like any iterative solution procedure, the iterative coupling also requires the use of a pre-determined tolerance value below which the solution if assumed to converge. Morita and Yen (2002) presents a set of models that are based on iterative coupling of surface and subsurface flows. According to their study, the earliest examples of iterative coupling were the studies by Pinder and Sauer (1971) and Freeze (1972a, b). In the surface flow component, both included the solution of one-dimensional dynamic wave equation along a rectangular channel. In the subsurface domain, Pinder and Sauer (1971) solved two-dimensional horizontal groundwater flow equations in the saturated medium where as Freeze (1972a, b) solved three-dimensional Richards equation in both unsaturated and saturated media. These studies are followed by Akan and Yen (1981a) where they solved one-dimensional dynamic wave equation for overland flow and two-dimensional Richards’ equation in unsaturated and saturated media. More recently, Govindaraju and Kavvas (1991) created an integrated model for hillslope hydrology, which included three flow pathways including a one-dimensional overland flow, a one-dimensional channel flow and a two-dimensional saturated/unsaturated subsurface flow component. A more complex simulation of overland flow is achieved by Bradford and Katopodes (1998) where they
solved two-dimensional turbulent Navier-Stokes equations for overland flow with two-dimensional Richards equation for groundwater flow. Recently, Morita and Yen (2002) developed a conjunctive two-dimensional surface and three-dimensional variably-saturated subsurface flow model by applying the two-dimensional non-inertia wave approximation of Saint-Venant equations in overland flow component and the three-dimensional Richards equation in unsaturated and saturated subsurface flow component.

In non-iterative (external) coupling, the surface and subsurface components are again solved separately at the same time step but in a non-iterative fashion. Even though the accuracy of solution from a non-iterative coupling technique is less than the solution from an iterative technique, this method found wide applicability among modelers due to its comparably less computational time requirements. In non-iterative coupling, the surface flow model is generally solved first in each time step and the results are passed to the subsurface flow model. Once the solution procedure of the subsurface component is completed at the same time step, the control is progressed to the next time step without entering an iterative loop where the model tries to satisfy the convergence of common flow variables such as overland flow water depth or infiltration flux. Numerous modelers have developed models with non-iterative coupling. One of the earliest of these studies is the one by Smith and Woolhiser (1971), where they solved one-dimensional kinematic wave equations for surface flow together with one-dimensional Richards’ equation for the unsaturated subsurface domain. Abbott et al. (1986a and 1986b) developed their well-known SHE model, which solved two-dimensional non-inertia wave equations for the overland flow and two-dimensional Richards’ equation for groundwater flow components. In a more recent study, Di Giammarco et al. (1994) combined two-dimensional overland flow equations, one-dimensional channel flow equations and one- and two-dimensional groundwater flow equations to obtain an integrated model for watershed runoff. Motha and Wigham (1995) also developed an externally coupled model of one-dimensional overland flow and two-dimensional subsurface flow. Wallach et al. (1997) studied the errors in surface runoff prediction by neglecting the relationship between infiltration rate and overland flow depth. They applied a kinematic wave approximation of Saint-Venant equations in their surface flow components and coupled it with two-dimensional Richards’ equation in their subsurface flow component. El-Hames and Richards (1998) combined three one-dimensional models of channel flow, overland flow and subsurface flow. They have used full dynamic wave equations in channel flow, kinematic wave equations in overland flow and Richards’ equation in subsurface flow. Similarly, Singh and Bhallamudi (1998) have coupled a one-dimensional dynamic wave model of overland flow with a two-dimensional subsurface flow model based on Richards equation.

Finally, the sink function type coupling is regarded as a further simplification to non-iterative coupling where infiltration is now considered as a sink for surface flow component. The one-dimensional downward movement of infiltration is modeled by using a semi-empirical algebraic equation such as Horton, Philip or Green and Ampt formula. Generally, the subsurface flow is not even modeled with models that apply sink function type coupling. In rare cases where it is modeled, infiltration is included as a source to groundwater flow. In this regard, it is clear that there is no direct link between surface and
subsidiary components and sink function type coupling is therefore known as “no-coupling” approach. Due to its computational ease, there exist many models that used sink function type coupling. Both Akanbi and Katopoulos (1988) and Playan et al. (1994) used two-dimensional non-inertia wave equations in surface flow component and Kostiakov equation in the infiltration sink function. Singh and Bhallamudi (1996) used one-dimensional dynamic wave equation in surface flow component and Kostiakov equation in infiltration function. On the other hand, Esteves et al. (2000), Yan and Kahawita (2000) and Tayfur et al. (1993) used Green and Ampt formula to model infiltration in their two-dimensional overland flow models. In three large scale applications, James and Kim (1990), Julien et al. (1995) and Chang et al. (2000) also used Green and Ampt infiltration equation to model two-dimensional overland flow but applied the non-inertia wave approximation to Saint-Venant equation to reduce computational costs.

Most of the time, the selection of the coupling technique is based on limitations of computational and data resources as well as the objectives of the study. Iterative coupling methods require significantly higher computational run-times when compared to non-iterative and sink function type coupling methods even to complete simulations of moderate time scales. The non-iterative and sink function type techniques reduce run-times by eliminating the necessity to iterate on model variables at each time step at the cost of reducing the model accuracy. In most cases where data is the limiting factor of the modeling effort, such reduction in accuracy is easily tolerated. It is often a dilemma of the modeler to choose between coupling techniques of higher accuracy and techniques that demand less data. Particularly for large scale modeling applications, this decision is biased towards techniques that require less data. In pilot or experimental scale studies, however, the modeler uses his luxury to implement models of high accuracy with unlimited data that he can collect from his ideal system. However, with the sophistication of remote sensing and geographic information systems, sophisticated coupling techniques started to become popular in large scale modeling efforts.

Apart from the coupling technique used, models of surface and subsurface flows are also classified according to the number of spatial dimensions used in discretizing the two flow domains. All surface flow models typically apply one- or two-dimensional discretization due to the relatively shallow water depths and well defined flow paths. In channel flows, modelers almost always prefer one-dimensional Saint-Venant equation or its approximations. In overland flows, both one and two-dimensional modeling is equally applied. The selection is mostly based on the complexity of the system under investigation and the available computer resources. Subsurface flow models, on the other hand, has a wide spectrum of spatial domain discretization. One-dimensional vertical flow models are mostly used with external and sink function type coupling techniques, where infiltration is mostly considered as a sink for overland flow phenomena. Two- and three-dimensional subsurface flow models are commonly applied with internal and simultaneous coupling methods.

Just like their discrete analogs, the coupled models also implement a wide array of numerical solution methods including the finite difference, finite element and method of
characteristics. The selection of the solution approach is based on: (i) the characteristics of the physical domain; (ii) number of spatial dimensions; (iii) ability to handle numerical problems; (iv) available computational resources; and, (v) the level of comfort the modeler feels with a particular technique.


2.5. Coupling of Transport Mechanisms

Despite the vast amount of literature describing the coupling of flow mechanisms, there is very limited source of information on how transport mechanisms of various domains must be linked together in a coupled modeling framework. It is the understanding of the author that coupled transport modeling is still a few steps behind its flow counterpart and there is a significant potential for development in this field. Only recently, a couple of studies has emerged describing some level of coupling of surface and subsurface transport processes including the works of Yeh et al. (1998), Ewen et al. (2000), Vanderkwaak and Loague (2001) and Lin and Medina (2003).
Since the information from the flow coupling such as the volumetric transfer rate is directly used in coupling transport processes, the coupling of transport mechanisms are done at exactly the same interfaces that flow coupling is carried out. Hence, the river bed, ground surface and water table are again used to link transport models to provide a continuous representation of the movement of a contaminant in the watershed. However, it is important to note that flow coupling must be executed smoothly and accurately before transport coupling could be attempted. The relatively immature level of flow coupling might explain to some degree about why researchers were hesitant to tackle the coupled transport problem.

Iterative and non-iterative coupling mechanisms are also used in linking contaminant transport in various domains. The idea behind coupling transport processes strictly follow flow coupling and relative heads are replaced by relative concentrations in different domains. The additional complication, however, arises from the nature of modeling transport processes and more sophisticated numerical algorithms with more computational requirements are generally necessary to obtain an equally accurate transport simulation.

2.6. Scale Issues

In a general definition, the term “scale” refers to the characteristic spatial or temporal dimensions at which entities, patterns, and processes can be observed and characterized to capture the important details of a hydrologic process. All hydrologic processes, large-scale or small-scale, have their own characteristic scales of reference, which is necessary to capture details of the processes modeled or observed. Independent of the size of the model used, all hydrologic models are based on some mathematical representation of a physical process which is scale dependent. When analysts use large-scale models to predict small-scale events, or when small-scale models are used to predict large-scale events, problems may arise. In the following sections, scale issues are discussed from a general perspective and specific details associated with subprocesses are presented in details. These sections closely follow the work of Aral and Gunduz (2003).

2.6.1. Fundamentals of Scales

From saturated-unsaturated groundwater flow and contaminant transport models to flow and transport in river channel networks, the hydrological processes occur at a wide range of scales and span about ten orders of magnitude in space and time. When an integrated system is modeled, the major question to be answered is whether to include all components of the hydrologic cycle into one system model. In a global sense, no component of the cycle could be separated from the overall system. However, the need for some artificial separation might be inevitable depending on the goals of the analysis and the importance of the contribution of the subprocess to the understanding and evaluation of that goal (Aral and Gunduz, 2003). In this regard, if one is not interested in observing or reflecting the effect of one subcomponent on the other, than one can easily isolate a hydrologic process and analyze that subcomponent alone. For example there are numerous groundwater flow and contaminant transport models which are extensively used in the literature just to study
groundwater systems such as the MODFLOW model of McDonald and Harbaugh (1998) and the SAINTS model of Aral (1990). In this type of an analysis, groundwater would consider some input/output from surface water but would not influence the conditions in the surface flow. On the other hand, if the simulation of multi-pathway interaction of hydrologic processes is the goal, than an integrated system modeling approach becomes a necessity and therein lay the difficulties of integration of scales.

The transfer of data or information across scales or linking sub-process models through a unified scale is referred to as “scaling” in the literature. Up-scaling consists of taking information at smaller scales to derive processes at larger scales, while downscaling consists of decomposing information at one scale into its constituents at smaller scales (Jarvis, 1995). In the context of absolute space and time, scaling primarily involves a change in the geometric and temporal structure of the data and their corresponding attributes. The term “absolute scale” refers to the definitions used in an Eulerian coordinate system where distances between points in time and space are well defined geometric and differential entities. Thus, linking sub-process parameters within these well defined rules can be considered to be objective and to be independent of one’s viewpoint or frame of reference in solving a problem. From the relative perspective, scaling becomes a more complex task than from the absolute framework. In the relative scale framework, one focuses on the sub hydrologic processes and defines the space and time as a measure of relationship between these sub-processes. In a way one can interpret this definition as a Lagrangian frame of reference. Relative scales concept represents the transcending concepts that link processes at different levels of space and time. It entails a change in scale that identifies major factors operational on a given scale of observation, their congruency with those on the lower and higher scales, and the constraints and feedbacks on those factors (Caldwell et al., 1993). With this definition, one can observe that two processes that occur in close proximity by the definition of an absolute scale may be very distant from one another in a relative scale sense. An example could be the case of the two hydrologic processes such as overland flow and saturated groundwater flow zones separated by an unsaturated zone. These two hydrologic processes could be close to each other in an absolute sense but in terms of their interaction with one another, these processes could be very distant from one another in relative space and time frame of reference due to limiting transfer rates that may exist in the unsaturated zone. In such cases, the relative frame of reference should take precedence when scaling is considered.

As expressed by Jarvis (1995), what makes scaling a real challenge is the non-linearity between processes and variables scaled, and the heterogeneity in properties that determines the rates of processes in a relative frame of reference. Therefore, it is important to realize that scaling requires an understanding of the complex hierarchical organization of the geographic and temporal worlds where different patterns and processes are linked to specific scales of observation, and where transitions across scales are based on geographically and temporarily meaningful rules (Marceau, 1999).

Scaling and its effects on hydrological modeling are commonly linked to heterogeneity of the system modeled. However, this link should also include the refinement necessary to
resolve the mathematical non-linearities incorporated into a hydrologic process. The importance of mathematical non-linearities can be clearly seen in the components of a sub-hydrologic model such as groundwater flow. Scale differences of saturated and unsaturated groundwater flow could be given as an example of this type of a problem. While dependence of hydraulic conductivity on saturation in the unsaturated zone is a major source of mathematical non-linearity that process introduces to the solution of the governing equation, spatially variable hydraulic conductivity of the saturated zone is a heterogeneity that needs to be addressed but does not significantly alter the solution characteristics of the governing equation. Thus, non-linearity and heterogeneity are the two important factors that need to be considered in scaling. The greater the degree of heterogeneity and non-linearity, the smaller the scale one would have to use to represent such variability or resolve such non-linearity (Aral and Gunduz, 2003).

The other component of scaling effect arises in the interpretation of field data. Integrated hydrologic models use a variety of parameters to represent the characteristics of a watershed. However, data on watershed parameters are only available at a limited number of locations. The task is then to transform this spatially limited data to a scale which can be used as input in a large scale watershed model. The problem then becomes the selection of a scale that can represent this data without losing accuracy during the extrapolation process. As the spatial scale of the model increases from a small area to a large area, the extrapolation of limited spatial data to a large scale system would introduce errors in the analysis from the start and should be avoided at all costs.

Singh (1995) defines scale as the size of a grid cell or sub-watershed within which the hydrologic response can be treated as homogeneous. If this scale is too small, the process will be dominated by local physical features, if this scale is too large, the process will ignore significant hydrologic heterogeneity caused by spatial variability. As much as this definition is correct and reasonable, it does not incorporate the scale effects associated with the resolution of mathematical non-linearity issues associated with an integrated modeling effort of the type considered here, i.e. integrated overland, channel and groundwater flow and contaminant transport in large scale watershed systems. An optimum scale of an integrated watershed model should then reflect the functional scale that provides a compromise between the resolution of non-linearities of the mathematical model, availability and extrapolation of hydrologic data and the heterogeneity of the system.

2.6.2. Scales of Watershed Subprocesses

Different scales of space and time govern the physical flow and transport phenomena in the hydrologic cycle. For integrated watershed models, these scales vary several orders of magnitudes in terms of the computational step size, the simulation extent that is necessary to capture the important aspects of the hydrologic process modeled as well as the proper scales that are necessary to interpret the input data.

In the unsaturated groundwater flow in the vertical domain, the movement of moisture is relatively slow when compared to other sub-processes of the hydrological cycle. Simulation
of this process is generally complicated by the existence of strong non-linearity in the properties of the medium for a large scale simulation. This non-linearity can be further complicated by the presence of a relatively dry medium where large hydraulic gradients may develop between the dry lower layers of the soil and the wet surface layers or visa versa. Hence, unsaturated zone modeling requires very small time and spatial discretization to handle both the strong non-linearity that often occur in layered soils and also to accurately capture the piston-like flow pattern at the wetting front. Small discretization is also essential for maintaining the water balance in a strongly non-linear system. In this regard, effective simulations in field applications in large watershed modeling typically require time and space scales in the order of $10^{-1}$-$10^2$ sec and $10^{-2}$-$10^1$ cm, respectively (Aral and Gunduz, 2003). This results in a system of very large number of nodes and time steps to simulate even a relatively small domain. Further complications might occur when modeling include processes such as root update and evaporation. To model such processes the scales may have to be further be refined to achieve numerically acceptable and physically sound results. In extreme case, it is possible that one might have to face almost real-time simulation run times, which is impractical from an engineering standpoint. Therefore, selecting a suitable spatial and temporal scale in unsaturated flow domain can become one of the most challenging tasks of the modeler.

The overland flow is another challenging sub-process of the hydrologic cycle. The problem in this domain is the continuity of flow in this phase. While there is continuous flow in all other sub-processes, the overland flow pattern is highly discontinuous in time. Its behavior is a strong function of the intermittent and spatially distributed source pattern (i.e. precipitation). Furthermore, it is a temporally relatively short event when compared to other flow processes such as river flow and groundwater flow. Thus, the overland flow may best be described as a moving boundary problem, which requires sophisticated numerical solution strategies (Aral and Gunduz, 2003). In this type of applications, discontinuities in time and space domains complicate the numerical solution of overland flow. Further difficulties arise from the small water depths associated with overland flow patterns. As a rule of thumb, it is highly uncommon to find overland flow depths larger than 2-3 cm, which produces small resistance coefficients (high resistance to flow). This characteristic of the flow combined with the strong, two-way and spatially-distributed interactions with the unsaturated zone might render the solution numerically unstable very easily. Additional complications of the overland flow occur due to tendency of overland flow to channelize making it extremely difficult to define the flow boundaries. These difficulties of overland flow as well as the time and space scales of the forcing function (i.e., precipitation) typical necessitate the use of $10^{-1}$ to $10^2$ sec time steps and $10^1$-$10^4$ cm spatial discretizations (Aral and Gunduz, 2003).

The saturated groundwater flow is perhaps the only sub-process that scale issues do not introduce extra complications for its solution. Since groundwater flow is slow when compared to surface flow processes such as river and overland flow, one can use very large time steps such as $10^3$-$10^6$ secs or even higher (Aral and Gunduz, 2003). The spatial scales would generally depend on the non-linearity of the medium but are generally large compared to other processes such as $10^3$-$10^6$ cm (Aral and Gunduz, 2003). However,
difficulties arise when the slowly moving groundwater flow is linked to other processes which are more dynamic. Therefore, it is possible to conclude that the numerical simulation of saturated groundwater flow can become extremely challenging when dynamic, real-time interactions with other sub-processes are included in an integrated model.

Finally, the river flow is the most dynamic flow pathway of the hydrologic cycle. In general, the simulation time scales are a strong function of the steepness of the hydrograph to be routed in the flow channel. Time steps of $10^2$-$10^5$ sec are used to simulate the flow patterns in moderate to large natural river networks (Aral and Gunduz, 2003). On the other hand, spatial scales are mostly a function of the channel characteristics including slope, flow cross section area and roughness coefficient. Spatial steps of $10^3$-$10^6$ cm are commonly used in simulations of gradually varied unsteady flow in river channels (Aral and Gunduz, 2003). Mainly due to the fact that the time and space scales are relatively large and mathematical procedures are well established, river flow modeling became well established within the overall watershed hydrology. Even with its current level of advancement, river models face challenging simulations particularly with steep hydrographs and highly non-linear channel geometries, which in turn might require that the space and time scales given above are modified radically.

2.7. Data Requirements

The data requirements of watershed models are one of the major issues that the hydrologic modeler has to focus on. Depending on the type of the model, these requirements might occasionally reach to such levels that it might totally destroy the effort. Particularly, the distributed watershed models are very costly in terms of the operational data requirements. Since such models are based on spatial variability of parameters over the watershed area, the input data is expected to be compatible and satisfy the needs of each model component. Therefore, the data requirements of all the subprocesses included in an integrated model should be studied in details at the earlier stages where model formulation is done. Unless satisfactory data resources are found, a decision to include a watershed process in the integrated model is subjective and would not make much sense.

The channel flow domain is amongst the few that data is easily accessible given enough resources. The major data requirement in the one-dimensional channel flow model is the characterization of the channel that would involve the analysis of channel topographic features (i.e., reach lengths, bottom elevations above a datum and slopes) and channel conveyance characteristics (i.e., tables relating water surface elevation to channel top width and roughness coefficients). Another crucial data requirement of channel flow model is the time dependent boundary condition data that drives the model. Access to stage and discharge hydrographs or stage-discharge rating curves is extremely important for accurate simulations of channel flow processes. Finally, reasonably accurate initial condition data is also important for successful start up of a model. Without such data, the numerical model could easily create stability problems which would eventually blow the simulation.
The major data requirement of the overland flow model is the description of the overland surface. This description includes a basic topographic characterization of the watershed surface (i.e., surface elevation, slope, orientation) and a specification of overland roughness coefficients based on land use/cover data. Another crucial data requirement of the overland flow analysis is the source function specification. Access to spatially and temporarily distributed precipitation data is of vital importance for the success of the overland flow simulations. Using remote sensing technology such as weather radars and satellites, it is now not difficult to supply this data to overland flow models. The boundary condition data is generally not very important in overland flow analysis when the majority of the flow boundaries are taken as watershed boundaries that enforce a zero flow depth. Only at the outflow boundary, the conditions must be carefully determined and imposed on the model. Finally, the initial condition data of the overland flow domain is mostly supplied by a zero depth condition along the entire watershed as long as flow is purely a function of precipitation input and there exists no prior overland water accumulation on the watershed.

In the saturated groundwater flow domain, the aquifer characteristics are the most significant data requirement. The modeler must have a clear understanding of the geological features of the aquifer and make sure that his representation of the system is a replica of the real situation in the field. Aquifer characterization would also involve the determination of the material properties of the aquifer (i.e., hydraulic conductivity and specific storage), without which, groundwater flow analysis is not possible. The specification of boundary conditions is another major data requirement that all groundwater flow models require. Time-dependent specification of specified head, specified flux or head-dependent boundary conditions must be done along the entire boundary of the modeling domain. Finally, a fairly accurate representation of initial hydraulic head is also crucial for successful modeling of groundwater flow pattern. However, the numerical solution of groundwater flow is generally more resistant to errors in initial conditions than channel flow models are.

The data requirements of the unsaturated zone groundwater flow model are very similar to the saturated zone. The material characteristics of the medium (i.e., the hydraulic conductivity and storage coefficient) are the major data source that must be supplied to any unsaturated zone model. The problem is generally more complicated compared to the saturated zone due to the additional difficulty arising from the dependency of model parameters to the saturation level in the domain. Therefore, the hydraulic conductivity values are to be quantified according to the level of saturation in the medium. When the relationships between soil-water parameters are not properly quantified using field data, approximate empirical models are to be used that reduces the level of accuracy of the results.
3. Coupled Flow Model

In this chapter, watershed scale flow pathways are analyzed within the context of a coupled system approach. The governing equations, initial and boundary conditions as well as the numerical solution schemes of each model component is first given to describe the physics of each flow pathway. Then, two possible coupled models of surface-subsurface flow processes are discussed comprehensively. A new simultaneous coupling methodology is proposed to solve the coupled system more accurately and with better representation of physical processes. The chapter concludes with the introduction of a ‘hybrid’ modeling concept to alleviate the difficulties of large scale, physically-based distributed watershed modeling.

3.1. One Dimensional Channel Flow Model

3.1.1. Governing Equations

The mathematical model of the one-dimensional channel flow is given by the continuity and momentum equations that are modified to include the effects of natural channel geometry and characteristics of rivers (Fread, 1993). In this study, the momentum equation is based on the complete dynamic wave form of the unsteady non-uniform St. Venant equations:

\[
\frac{\partial s_c (A + A_o)}{\partial t} + \frac{\partial Q}{\partial x} - q_{L1} - q_{L2} = 0
\]

\[
\frac{\partial s_m Q}{\partial t} + \frac{\partial (\beta Q^2/A)}{\partial x} + gA \left( \frac{\partial h_r}{\partial x} + S_f + S_{ec} \right) + M_{L1} + M_{L2} = 0
\]

where \( x \) is the longitudinal coordinate representing the distance along the channel/flood plain, \( t \) is the temporal coordinate, \( s_c \) and \( s_m \) are sinuosity factors for continuity and momentum equations, respectively, \( A \) is the active cross-sectional area of flow, \( A_o \) is the inactive (off-channel storage) cross-sectional area of the channel/floodplain, \( Q \) is the discharge, \( q_{L1} \) is the lateral seepage flow per channel length (positive for inflow and negative for outflow), \( q_{L2} \) is the lateral overland flow per channel length (positive for inflow and negative for outflow), \( \beta \) is the momentum coefficient for velocity distribution, \( g \) is the gravitational acceleration, \( h_r \) is the water surface elevation in the river (i.e., stage), \( M_{L1} \) is the momentum flux due to lateral seepage inflow/outflow, \( M_{L2} \) is the momentum flux due to lateral overland inflow/outflow; and, \( S_f \) and \( S_{ec} \) are channel/flood plain boundary friction slope and contraction/expansion slope, respectively. The momentum flux due to lateral seepage and overland flows, contraction/expansion slope and channel/flood plain boundary friction slope are evaluated as:
\[ M_{L_1} = \begin{cases} 
0 & \text{for seepage inflow} \\
-\frac{Q_{q_{11}}}{2A} & \text{for seepage outflow}
\end{cases} \quad (3.3) \]

\[ M_{L_2} = \begin{cases} 
-\beta v_x q_{L_2} & \text{for overland inflow} \\
-\frac{Q_{q_{12}}}{A} & \text{for overland outflow}
\end{cases} \quad (3.4) \]

\[ S_{ec} = \frac{K_r \Delta(Q/A)^2}{2g \Delta x} \quad (3.5) \]

\[ S_f = \frac{n_c^2 |Q/Q|}{c_1^2 A^2 R_h^{4/3}} = \left| \frac{Q/Q}{K^2} \right| \quad (3.6) \]

where \( v_x \) is the velocity of the overland flow in the direction of channel flow, \( K_{ec} \) is the expansion/contraction coefficient, \( \Delta x \) is the reach length, \( c_1 \) is a unit system dependent constant (i.e., 1.0 in SI unit system and 1.486 in British unit system), \( n_c \) is the Manning’s roughness coefficient in river channel, \( K \) is the flow conveyance factor and \( R_h \) is the hydraulic radius. The hydraulic radius is defined as the ratio of cross-sectional area to wetted perimeter but is approximated in this study as the ratio of cross-sectional area to top width for large rivers. The lateral flow that provides the link between the channel flow model and the saturated groundwater flow model is defined as:

\[ q_{L_1} = \begin{cases} 
-K_r w_r \frac{h_r - h_g}{m_r} & h_g > (z_r - m_r) \\
-K_r w_r \frac{h_r - (z_r - m_r)}{m_r} & h_g \leq (z_r - m_r)
\end{cases} \quad (3.7) \]

where \( K_r \) is the river bottom sediment hydraulic conductivity, \( m_r \) is the thickness of river bottom sediments, \( z_r \) is the river bottom elevation, \( w_r \) is the wetted perimeter of the river bed and \( h_g \) is the groundwater hydraulic head. The details of the coupling between river and groundwater flow systems are given in Section 3.5.1.

### 3.1.2. Initial Conditions

In order to start the transient solution, initial values of the unknowns (i.e., discharge and water surface elevation) are to be specified along the one-dimensional channel domain. The initial conditions can be obtained from: (i) field data; (ii) a previous unsteady model solution; or, (iii) solution of steady, non-uniform flow equation. In any case, the initial conditions are given as:

\[ Q(x,0) = Q_0(x) \quad (3.8) \]

\[ h_r(x,0) = h_{r0}(x) \quad (3.9) \]
where \( Q_0 \) and \( h_{r0} \) represent the discharge and water surface elevation in the channel at the beginning of the simulation, respectively.

3.1.3. Boundary Conditions

In the one-dimensional channel flow model, there are two different types of boundary conditions specified at: (i) external; and, (ii) internal boundaries of the domain. The external boundary conditions are given at the most upstream and downstream points of the channel network where as the internal boundary conditions are specified at internal junction points of the channel network.

3.1.3.1. External Boundary Conditions

In this study, the proposed model is capable of modeling a network of river channels. The tree-like network is composed of several upstream and internal channels and a single downstream channel. Therefore, the model can accommodate several upstream boundary conditions and a single downstream boundary condition. In this regard, the model does not solve looped channel networks. At any upstream boundary, a discharge or a stage hydrograph can be used as the boundary condition. These conditions are expressed as discharge and stage time series and are given as:

\[
Q(0,t) = Q_u(t) \quad (3.10)
\]
\[
h_r(0,t) = h_u(t) \quad (3.11)
\]

where \( Q_u \) and \( h_u \) represent upstream boundary discharge and water surface elevation values, respectively. Similarly, the boundary condition at the downstream boundary can also be defined as a discharge or a stage hydrograph and specified as:

\[
Q(L_d,t) = Q_d(t) \quad (3.12)
\]
\[
h_r(L_d,t) = h_d(t) \quad (3.13)
\]

where \( Q_d \) and \( h_d \) represent downstream boundary discharge and water surface elevation values, and \( L_d \) is the total domain length. In addition, it is also possible to define the downstream boundary condition as a single-valued rating curve, a looped rating curve or a critical depth section. The single-valued rating curve maps a particular stage value to a corresponding discharge value and can be expressed by using linear interpolation within a table of stage-discharge data:

\[
Q(L_d,t) = Q^k + \frac{Q^{k+1} - Q^k}{h_r^{k+1} - h_r^k} (h_d - h_r^k) \quad (3.14)
\]
where $Q^k, Q^{k+1}, h_r^k$ and $h_r^{k+1}$ are consecutive tabular data sets of the rating curve and $h_d$ is the stage at the downstream boundary. A looped rating curve, on the other hand, maps a stage value to several possible discharge values depending on the hydraulic conditions of the channel and can be expressed using the Manning’s equation:

$$Q(L_d, t) = \frac{c_1}{n_c} A R_h^{2/3} S_f^{1/2}$$

where $S_f$ is given by the modified momentum equation as:

$$S_f = -\frac{1}{gA} \frac{\partial Q}{\partial t} - \frac{1}{gA} \frac{\partial(Q^2 / A)}{\partial x} - \frac{\partial h_r}{\partial x}$$

Finally, it is also possible to use critical depth as the downstream boundary condition when the most downstream point of the modeling domain is a controlled structure such as a weir. In this particular case, the critical depth is mapped to the critical discharge via the following equation:

$$Q(L_d, t) = \sqrt{\frac{g}{B}} A^{3/2}$$

where $B$ is the cross-sectional top width of the channel.

3.1.3.2. Internal Boundary Conditions

Any two or more channels intersecting within a channel network forms a junction where internal boundary conditions are specified to satisfy the mass and energy balance. In this study, the proposed model does not allow for looped networks and require that there is always a single outflow channel from a junction. The mass balance equation at a junction can therefore be specified as:

$$\sum_{k=1}^{m} Q_k - Q_o = \frac{dS}{dt}$$

where $m$ is the total number of inflowing channels to the junction, $Q_k$ is the discharge at the end of the $k^{th}$ inflowing channel to the junction, $Q_o$ represents the discharge at the beginning of the outflowing channel from the junction, and $dS/dt$ corresponds to the change in storage within the junction. For many modeling applications, it is a common practice to assume that the change in storage within a junction is negligible compared to the change in storage within in a channel (Akan and Yen, 1981b; Fread, 1993; Jha et al., 2000). Consequently, the mass balance equation reduces to a simple continuity equation. On the other hand, the energy equation at a junction is written as:
where \((h_r)_k\) and \(V_k\) are the stage and flow velocity at the end of the \(k\)th inflowing channel to the junction, \((h_r)_o\) and \(V_o\) are the stage and flow velocity at the beginning of the outflowing channel from the junction and \(h_T\) is the total headloss in the junction. When all the flows in all the branches joining a junction are subcritical and the head lost in the junction is negligible, the equation simplifies to:

\[
(h_r)_k = (h_r)_o \quad k = 1,2,\ldots,m
\]  

and is commonly used in modeling channel networks (Akan and Yen, 1981b; Fread, 1993; Jha et al., 2000).

### 3.1.4. Numerical Solution Scheme

In general, the available numerical techniques for the solution of expanded Saint-Venant equations can be given as: (i) method of characteristics; (ii) finite difference methods; and, (iii) finite element methods. Of these methods, the finite element method is rarely used when flow is approximated as one-dimensional such as in the case of Saint-Venant equations. The other two methods have been commonly applied for the numerical solution of one-dimensional unsteady flow since 1960s. The finite difference methods can further be classified as explicit and implicit techniques, each of which holds distinct numerical characteristics. A major advantage of the implicit finite difference method over the method of characteristic and the explicit finite difference technique is its inherent stability without the requirement to satisfy the Courant condition, which sets the criteria for the maximum allowable time step. This requirement to satisfy Courant condition often makes the method of characteristics and explicit techniques very inefficient in terms of the use of computer time. Furthermore, certain implicit schemes such as the one proposed by Preissmann (1961) allow the use of variable time and spatial steps, which make the method extremely convenient for applications in routing of flood hydrographs in river systems (Sturm, 2001). Considering these advantages, the implicit finite difference technique is used to solve the channel flow equations given by equations (3.1) and (3.2).

Of the various implicit schemes that have been developed, the "weighted four-point" scheme of Preissmann is very valuable since it can readily be used with unequal distance steps that becomes particularly important for natural waterways where channel characteristics are highly variable even in short distances. Similarly, the applicability of unequal time steps is another important characteristic of this technique for hydrograph routing where floodwaters would generally rise relatively quickly and recess gradually in time.

The finite difference counterparts of the continuity, momentum and boundary condition equations are given in Gunduz (2004). In a channel network, the discretized forms of
equations (3.1) and (3.2) form the core of the channel flow model. These equations are written for each channel in the network, and supplemented by the discretized forms of the boundary condition equations. For each channel, the final form of the continuity equation written for an intermediate node is given as:

\[
\frac{\Delta x_i}{2\Delta t_i} \left[ s_{c,i+1/2}^{j+1} (A + A_o)^{j+1}_{i+1/2} + s_{c,i+1/2}^{j+1} (A + A_o)^{j+1}_{i} - s_{c,i+1/2}^{j} (A + A_o)^{j}_{i+1/2} - s_{c,i+1/2}^{j} (A + A_o)^{j}_{i} \right] \\
+ \theta_f \left[ Q_{r,i+1}^{j+1} - Q_{r,i}^{j+1} - \Delta x_i \left[ \left( -\frac{K_r w_r}{m_r} \right)^{j+1}_{i+1/2} \left( h^{j+1}_{r,i+1/2} - h^{j+1}_{s,i+1/2} \right) - \Delta x_i (q_{L2,i+1/2})^{j+1} \right] \right] - (3.21)
\]

\[
+ (1 - \theta_f) \left[ Q_{r,i}^{j+1} - Q_{r,i}^{j} - \Delta x_i \left[ \left( -\frac{K_r w_r}{m_r} \right)^{j}_{i+1/2} \left( h^{j}_{r,i+1/2} - h^{j}_{s,i+1/2} \right) - \Delta x_i (q_{L2,i+1/2})^{j} \right] \right] = 0
\]

Similarly, the finite difference form of the momentum equation written for an intermediate node is given as:

\[
\frac{\Delta x_i}{2\Delta t_i} \left[ s_{m,i+1/2}^{j+1} Q_{r,i+1}^{j+1} + s_{m,i+1/2}^{j+1} Q_{r,i}^{j+1} - s_{m,i+1/2}^{j} Q_{r,i+1}^{j} - s_{m,i+1/2}^{j} Q_{r,i}^{j} \right] \\
+ \theta_f \left[ \left( \beta Q^2 / A \right)^{j+1}_{i+1/2} \left( \beta Q^2 / A \right)^{j+1}_{i} + g A_{s,i+1/2}^{j+1} h^{j+1}_{r,i+1/2} + \Delta x_i S_{f,i+1/2}^{j+1} + \Delta x_i S_{e,i+1/2}^{j+1} \right] \\
+ \Delta x_i (M_{L1})^{j+1}_{i+1/2} + \Delta x_i (M_{L2})^{j+1}_{i+1/2} \\
+ (1 - \theta_f) \left[ g A_{s,i+1/2}^{j} h^{j}_{r,i+1/2} + \Delta x_i S_{f,i+1/2}^{j} + \Delta x_i S_{e,i+1/2}^{j} \right] + \Delta x_i (M_{L1})^{j}_{i+1/2} + \Delta x_i (M_{L2})^{j}_{i+1/2} = 0
\]

where corresponding formulations developed in Gunduz (2004) are substituted for the slope terms $S_f$ and $S_{sec}$, as well as the lateral flow terms $M_{L1}$ and $M_{L2}$. In equations (3.21) and (3.22), subscripts $i$ and $j$ represent the spatial and temporal indices, respectively. The terms with subscript $j$ are known either from initial conditions or from the solution of Saint-Venant equations at the previous time line. Since cross sectional area and channel top width are functions of water surface elevation, the only unknown terms in these equations are discharge and water surface elevation at the $(j+1)^{th}$ time line at nodes $(i)$ and $(i+1)$. Therefore, there are only four unknowns in these two equations. All remaining terms are either constants or are functions of these unknowns. The resulting two algebraic equations obtained by the application of the weighted four-point scheme are nonlinear and an iterative solution technique is required.
When the finite difference forms of continuity and momentum equations are solved for each channel grid shown in Appendix A of Gunduz (2004), a system of $2(N_k-1)$ equations are formed for one time-line between the upstream and downstream boundary of channel $k$, where $N_k$ represents the number of nodes in channel $k$. The two unknowns in each of these equations yield a total of $2N_k$ unknowns for each time line. The system of $2(N_k-1)$ equations with $2N_k$ unknowns requires two additional equations for the closure of the system. These two additional equations are supplied by the upstream and downstream boundary conditions of the channel. The discretized forms of these equations are also presented in Gunduz (2004). When this procedure is repeated for each channel of the network, a total of $\Sigma(2N_k)=2N$ equations are formed, where $k$ runs from 1 to the number of channels in the network, and $N$ represents the total number of nodes in the entire system. The resulting system of $2N$ non-linear equations with $2N$ unknowns is solved by a suitable non-linear matrix solution algorithm.

Of all the non-linear solution procedures, the Newton-Raphson method is one of the most common iterative techniques used for the solution of a system of non-linear equations. It provides an efficient means of converging to a root given a sufficiently good initial guess. For any channel network application, the system of equations can be denoted as $2N$ functional relations to be zeroed that involves variables $Q$ and $h_r$ represented by $x_k$ for $k=1,2,...,2N$:

$$f_k(x_1, x_2, x_3,..., x_{2N}) = 0$$  \hspace{1cm} (3.23)

If $x$ denotes the entire vector of unknown variables $x_k$ and $f$ denotes the entire vector of functions $f_i$, each of the functions $f_i$ can be expanded as a Taylor series expansion in the neighborhood of $x$:

$$f_k(x + \delta x) = f_k(x) + \sum_{m=1}^{2N} \frac{\partial f_k}{\partial x_m} \delta x_m + O(\delta x^2)$$  \hspace{1cm} (3.24)

where the matrix of first partial derivatives is called the Jacobian matrix, $J$. The elements of the Jacobian matrix for $2N$ unknowns are evaluated in Gunduz (2004). In matrix notation, one can rewrite equation (3.24) as:

$$f(x + \delta x) = f(x) + J \cdot \delta x + O(\delta x^2)$$  \hspace{1cm} (3.25)

Neglecting the higher order terms and setting the left hand-side equal to zero, one can obtain a set of linear equations that is written as:

$$J \cdot \delta x = -f$$  \hspace{1cm} (3.26)

This matrix equation is solved by a suitable matrix solver for the unknown $\delta x$, and an improved estimate of solution is obtained by:
\[ x^{j+1,k+1} = x^{j+1,k} + \delta x^{j+1,k} \]  

(3.27)

where superscript \( k \) represents the level of iteration at the unknown time line. The iterative solution is tracked by finding the values of the unknowns \( Q \) and \( h_r \) so that the residuals given in equation (3.27) are forced to zero or very close to zero. It must be noted that the convergence process depends on a good first estimate for the unknown variables. Fread (1985) states that a reasonably good estimate for the first time step is to use the initial condition of discharge and water surface elevation. For all other time steps, the first estimates of the unknown variables can be obtained by using the linearly extrapolated values from solutions at previous time steps according to the algorithm given below:

\[ x^{j+1,1} = x^j + \alpha_c (x^j - x^{j-1}) \frac{\Delta t^{j+1}}{\Delta t^j} \quad j \neq 1 \]  

(3.28)

where \( x^{j+1,1} \) is the first estimate of unknown variables at \((j+1)\)th time line, \( x^j \) is the solution vector of \( Q \) and \( h_r \) values from previous time step, \( x^{j-1} \) is the solution vector of \( Q \) and \( h_r \) values from two previous time steps, \( \alpha_c \) is a weighing factor from 0 to 1 and \( \Delta t^{j+1} \) and \( \Delta t^j \) are the two consecutive time step sizes.

3.1.5. Model Testing

The channel flow model is one of the most complicated partial differential equations in the computational fluid dynamics area. Since there are no known analytical solutions to the coupled continuity and momentum equations, the proposed model is tested against the popular HEC-RAS river analysis software developed by the U.S. Army Corps of Engineers Hydrologic Engineering Center (Brunner, 2002) and the previously published model of Choi and Molinas (1993).

Three tests are done to check the performance of the proposed model. In the first test, a triangular flood hydrograph is routed in a single channel. The 10000m long channel is rectangular in cross-section with a constant width of 20m and lies on the slope 0.001 m/m. A Manning’s roughness coefficient of 0.020 is used throughout the channel. At the upstream boundary, the discharge hydrograph is used as the boundary condition. At the downstream boundary, a constant water depth of 2m is used throughout the simulations. The simulations are made with a constant grid spacing of 100m and a time step of 1hr. For this particular example, the results of the proposed model are compared with the results from both the HEC-RAS model. Comparisons are made at the mid-point of the channel and at the most downstream point of the channel. The results of the comparison are given in figures 3.1 and 3.2.
Figure 3.1. Comparison of single channel simulations at mid-point cross-section
Figure 3.2. Comparison of single channel simulations at most downstream cross-section
As seen from figures 3.1 and 3.2, the proposed model and HECRAS results are identical to each other both at the mid-point of the channel and at the most downstream point of the channel. Therefore, the proposed model is shown to simulate a single channel case correctly by propagating and attenuating the triangular discharge hydrograph.

In the second test, a simple channel network is simulated with the proposed model as well as the HEC-RAS model. The network contains 2 upstream channels, a junction and a downstream channel (Figure 3.3). The upstream channels are 10000m and 5000m long respectively and have a slope of 0.001m/m. The downstream channel is 10000m long and have slope of 0.001m/m. All channels have a roughness coefficient of 0.030. The channels are trapezoidal in cross-section with a base width of 10m and a side slope of 2 to 1. At the upstream boundaries of the upstream channels, a single and double peaked triangular discharge hydrographs are used as the boundary conditions. At the most downstream point of the channel system, a constant water depth of 2m is used throughout the simulations. The simulations are made with a constant grid spacing of 100m and a time step of 1hr. Comparisons are made at the mid-point and at the exit point of the downstream channel. The results are given in figures 3.4 and 3.5.

![Figure 3.3. Simple network setup](image-url)
Figure 3.4. Comparison of simple network simulations at mid-point cross-section of downstream channel
Figure 3.5. Comparison of simple network simulations at most downstream cross-section
The proposed model is computed to give very close values to the HECRAS model. The deviations in peaks and depressions are mainly due to the hydraulic radius evaluation differences in these two models. In the proposed model, the wetted perimeter of a cross-section is approximated with the top width which makes it only an estimate for hydraulic radius evaluation where as HECRAS uses an exact evaluation method for the wetted perimeter and the hydraulic radius. The approximate procedure implemented in the proposed model is a widely applied technique for modeling real river systems (Fread, 1985; Fread, 1993; Jha et al., 2000). It may, however, create some discrepancies for applications to artificial channels where wetted perimeter is significantly different from the top width. Except for this approach problem, the two models practically generate identical results in terms of hydrograph timing.

The final test is taken from Choi and Molinas (1993) who analyzed a hypothetical dendritic system composed of five tributary channels and three main channels (Figure 3.6). A linear discharge variation with a maximum discharge of 2300ft³/s is used as the upstream boundary condition of all tributary channels. The tributary and main channel lengths were taken as 6mile long. The channel widths varied from 100ft for tributaries to 200ft for the reach downstream from tributaries 1 and 2, 400ft for the reach downstream of tributaries 3 and 4, to 500ft for the downstream main channel. The slope in each channel segment was taken to be 0.002ft/ft and the Manning’s roughness coefficient was 0.04. The initial discharge per unit width was constant throughout the network. The simulations were performed with 10min time increments and 1mile spatial spacing. For the initial conditions, the same water depths are assumed in all branches and in the main channel. Comparisons are made at the most downstream point of the channel network. The results from the proposed model and HEC-RAS are overlaid on Choi and Molinas’ results and are presented in Figure 3.7. Since Choi and Molinas did not provide a detailed output of their results, an overlay technique is used to compare the results of their model with the proposed model and HECRAS. In their study, they compare their dendritic model to sequential kinematic and sequential dynamic models and show that their dendritic model is capable of producing similar results. Comparisons of the proposed model, HECRAS and their dendritic model do not provide a definite bias towards a particular model. The proposed model, however, closely follows the results from the Choi and Molinas’ dendritic model in the early parts of the rising limb of the hydrograph during which the HECRAS significantly creates a delay in the arrival of the rising limb. The proposed model then shows signs of delay in the later parts of the hydrograph rising limb and slightly creates a delayed peak value when compared to the Choi and Molinas model and HECRAS. In the falling limb, however, the proposed model closely follows Choi and Molinas’ dendritic model as well as HECRAS. In terms of the value of the peak, the proposed model estimates very closely to Choi and Molinas’ model where as HECRAS slightly overestimates. An overall analysis of the results shown in Figure 3.7 reveal that the proposed channel flow model performs accurately compared to some other models. Exact comparisons are only possible with analytical solutions of the mathematical model that are currently not available.
Figure 3.6. Choi and Molinas (1993) dendritic network setup
3.2. Two Dimensional Saturated Groundwater Flow Model

3.2.1. Governing Equations

The governing equation of two-dimensional vertically-averaged saturated groundwater flow is obtained by vertically integrating the general three-dimensional conservation of mass and momentum equations describing subsurface flow (Aral, 1990). The equation is later on modified by Gunduz and Aral (2004a) to include the effect of line source/sink. For an anisotropic, non-homogeneous unconfined aquifer with principle permeability directions not matching the coordinate directions, the governing equation of vertically-averaged saturated groundwater flow is given by:
\[
S_y \frac{\partial h_g}{\partial t} - \frac{\partial}{\partial x} \left[ (h_g - z_b) (K_g)_{xx} \frac{\partial h_g}{\partial x} + (h_g - z_b) (K_g)_{xy} \frac{\partial h_g}{\partial y} \right] \\
- \frac{\partial}{\partial y} \left[ (h_g - z_b) (K_g)_{yx} \frac{\partial h_g}{\partial x} + (h_g - z_b) (K_g)_{yy} \frac{\partial h_g}{\partial y} \right] + \sum_{k=1}^{n} \left[ Q_{w,k} \delta (x - x_{w,k}) \delta (y - y_{w,k}) \right] \tag{3.29} \\
+ \sum_{m=1}^{n_r} \int_0^1 \left[ \frac{dg_{x,m}}{du} \right]^2 + \left[ \frac{dg_{y,m}}{du} \right]^2 \delta (x - g_{x,m}(u)) \delta (y - g_{y,m}(u)) du \right] + I = 0
\]

where \( x \) and \( y \) are the spatial coordinates in the horizontal domain, \( t \) is the temporal coordinate, \( S_y \) is the specific yield of the unconfined aquifer, \( h_g \) is the vertically-averaged hydraulic head, \( z_b \) is the top elevation of bottom impervious layer, \( K_g \) is the anisotropic saturated hydraulic conductivity, \( n_w \) is the number of wells in the domain, \( Q_{w,k} \) is the well flow rate of the \( k \)th well located at \((x_{w,k}, y_{w,k})\) in the domain (i.e., positive for a discharging well and negative for an injecting well), \( \delta \) is the Dirac Delta function, \( n_r \) is the number of river channels in the domain, \( q_{L1} \) is the lateral flow at the river-bottom interface defined by equation (3.7) (i.e., positive for lateral outflow from the aquifer and negative for lateral inflow to the aquifer), \( g_{x,m} \) and \( g_{y,m} \) are the Cartesian coordinate components of the parametric equation defining the \( m \)th river channel in the domain, \( u \) is the dimensionless parameter of the parametric equation and \( I \) is the infiltration/exfiltration rate (i.e., positive for exfiltration and negative for infiltration).

In general, the directions of the hydraulic conductivity measurements (i.e., the principle coordinate system) are different from the assumed global coordinate system on which the entire analysis is based on. Under such circumstances, a transformation is necessary to make proper use of the hydraulic conductivity data obtained from field studies. Hence, if the values of hydraulic conductivity are known in the principle coordinate system \((\xi, \eta)\), then their corresponding values in a global coordinate system \((x,y)\) making an angle \( \theta_c \) with the principle coordinate system are given as (Bear, 1979):

\[
(K_g)_{xx} = \frac{(K_g)_{\xi\xi} + (K_g)_{\eta\eta}}{2} + \frac{(K_g)_{\xi\eta} - (K_g)_{\eta\xi}}{2} \cos 2\theta_c \\
(K_g)_{yy} = \frac{(K_g)_{\xi\xi} + (K_g)_{\eta\eta}}{2} - \frac{(K_g)_{\xi\eta} - (K_g)_{\eta\xi}}{2} \cos 2\theta_c \\
(K_g)_{xy} = \frac{(K_g)_{\xi\xi} - (K_g)_{\eta\eta}}{2} \sin 2\theta_c \tag{3.30}
\]

3.2.2. Initial Conditions

The initial values of the hydraulic head, \( h_{gb} \), are specified as the initial conditions of the groundwater flow model:
\[ h_g(x, y, 0) = h_{g0}(x, y) \]  

which can be obtained from: (i) field measurements, (ii) a steady state flow simulation; and, (iii) a previous unsteady model solution.

3.2.3. Boundary Conditions

Three different types of boundary conditions can be specified along different external boundaries of the groundwater flow domain. Type-1 or specified head boundary conditions are used to model boundaries with known hydraulic head values. It is also known as a Dirichlet boundary condition and is given as:

\[ h_g(x, y, t) = h_{gD}(x, y, t) \]  

where \( h_{gD} \) is the known hydraulic head value. Type-2 or specified flux boundary conditions are used to model boundaries with known flux values. It is also known as a Neumann boundary condition and is given as:

\[ q_N(x, y, t) = -n \cdot \left((h_g - z_b) \cdot K_g \cdot \nabla h_g\right) \]  

where \( q_N \) is the known flux value and \( n \) is the unit normal to the boundary. Finally, type-3 or head-dependent boundary conditions are used to model boundaries on which the conditions depend on the changing hydraulic head such as streams, rivers or lakes at the external boundaries of the domain. It is also known as a Cauchy boundary condition and is given as:

\[ q_C(x, y, t) = -n \cdot \left((h_g - z_b) \cdot K_g \cdot \nabla h_g\right) = \begin{cases} -K_r w_r \frac{h_r - h_g}{m_r} & h_g > (z_r - m_r) \\ -K_r w_r \frac{h_r - (z_r - m_r)}{m_r} & h_g \leq (z_r - m_r) \end{cases} \]  

where \( q_C \) is the head-dependent flux value and is similar to the lateral seepage flow term defined internally in the domain and given in equation (3.7).

3.2.4. Numerical Solution Scheme

In groundwater flow modeling literature, there exist numerous models implementing different numerical solution procedures. The most common of these procedures are the finite difference and finite element methods (Narasimhan and Witherspoon, 1977; Huyakorn et al., 1986; McDonald and Harbaugh, 1998; Aral, 1990; Yeh, 1999; Morita and Yen, 2002). The finite element method became a popular method due to the flexibility it
offers in simulating large scale aquifer domains with irregular boundaries as well as heterogeneous aquifer properties. In this regard, the Galerkin finite element method based on the method of weighted residuals is used in this study to solve the groundwater flow.

The numerical procedure starts with the idealization of the solution domain by a finite number of distinct, non-overlapping regions, called the finite elements, over which the unknown variables are to be interpolated. In any idealization, the elements are selected such that the material properties of the domain, such as hydraulic conductivity and specific yield, are retained in individual elements. In two-dimensional finite element analysis, families of triangular and/or quadrilateral elements are generally used to discretize the analysis domain. Although these elements can be linear, quadratic or cubic, using simple linear elements generally provides sufficient accuracy and a better solution strategy. Quadrilateral elements are superior as opposed to triangular elements due to the fact that they are computationally more efficient and they simplify the task of tiling the problem domain without introducing any bias that the triangular elements possess. For these reasons, linear irregular quadrilateral elements with four nodes are selected to discretize the domain and develop basis functions in this study. The details associated with the basis functions are given in Gunduz (2004).

Following the idealization of domain and selection of the interpolating functions, an appropriate weak form of the problem is developed using the Galerkin weighted residual method as shown in Gunduz (2004) by using the standard steps of writing the weighted residual, integration by parts and incorporating the natural boundary conditions. The resulting finite element matrix equation obtained by applying the Galerkin procedure is given as:

$$ F_h = M \cdot \frac{d \hat{h}_g}{dt} + S \cdot \hat{h}_g $$  \hspace{1cm} (3.35)

where $S$, $M$ and $F$ stand for global stiffness matrix, global mass matrix and global load vector, respectively, and $\hat{h}_g$ is the approximate hydraulic head vector. These global matrices and vectors are obtained by tiling their element counterparts according to the connectivity of elements within the solution domain. The explicit formulations of element matrices and vectors are derived in Gunduz (2004). At this point, it is clearly seen that these element integrals are generally complex and cannot be integrated analytically. Hence, a numerical integration scheme is required to evaluate these element integrals. In this study, a two-dimensional Gaussian quadrature technique is implemented to evaluate these integrals numerically. The details of this technique are discussed in Gunduz (2004).

The ordinary differential equation (3.35) obtained as a result of finite element discretization could be solved using a number of techniques including the one-step finite difference approximations. Since the hydraulic head is a function of time, it is possible to define two positions, $j$ and $j+1$, representing the known and unknown time lines, respectively. If one
defines an intermediate point between the known and the unknown time line (i.e., \(j + \alpha\) where \(0 \leq \alpha \leq 1.0\)), then the corresponding head could be calculated as a weighted average:

\[
\hat{h}_g^{j+\alpha} = \alpha \hat{h}_g^{j+1} + (1 - \alpha) \hat{h}_g^j
\]

(3.36)

such that if the intermediate point is selected as the mid point between the two time lines (i.e., \(\alpha = 0.5\)), the head becomes an arithmetic average of the two heads at two ends. When the Taylor series expansion of the hydraulic head around the intermediate point is done using the points \(j\) and \(j+1\), one would obtain:

\[
\hat{h}_g^{j+(1-\alpha)} = \hat{h}_g^j + \left(1 - \frac{\alpha}{1!}\right) \Delta t \frac{\partial \hat{h}_g^j}{\partial t} + \frac{(1 - \alpha)^2}{2!} \Delta t^2 \frac{\partial^2 \hat{h}_g^j}{\partial t^2} + O(\Delta t^3)
\]

(3.37)

\[
\hat{h}_g^{j+(1-\alpha)} = \hat{h}_g^{j+1} - \frac{\alpha}{1!} \Delta t \frac{\partial \hat{h}_g^{j+1}}{\partial t} + \frac{\alpha^2 \Delta t^2}{2!} \frac{\partial^2 \hat{h}_g^{j+1}}{\partial t^2} - O(\Delta t^3)
\]

(3.38)

Neglecting the terms equal to or higher than second order and subtracting the second equation from the first yields:

\[
0 = \hat{h}_g^j - \hat{h}_g^{j+1} + (1 - \alpha) \Delta t \frac{\partial \hat{h}_g^j}{\partial t} + \frac{\alpha \Delta t}{1!} \frac{\partial \hat{h}_g^{j+1}}{\partial t}
\]

(3.39)

and after rearranging, reduces to:

\[
\frac{\hat{h}_g^{j+1} - \hat{h}_g^j}{\Delta t} = (1 - \alpha) \frac{\partial \hat{h}_g^j}{\partial t} + \alpha \frac{\partial \hat{h}_g^{j+1}}{\partial t}
\]

(3.40)

Since it is always possible to write the ordinary differential equation for a particular time line, one would obtain the following equations for the two time lines:

\[
S^j \cdot \hat{h}^j + M^j \cdot \frac{d \hat{h}_g^j}{dt} = F^j
\]

(3.41)

\[
S^{j+1} \cdot \hat{h}^{j+1} + M^{j+1} \cdot \frac{d \hat{h}_g^{j+1}}{dt} = F^{j+1}
\]

(3.42)

When these equations are multiplied by the weighing parameters \((1-\alpha)\) and \(\alpha\), respectively and added together, one would obtain:
\[ \alpha S^{j+1} \cdot \hat{h}_g^{j+1} + (1 - \alpha) S^j \cdot \hat{h}_g^j + \alpha M^{j+1} \cdot \frac{d\hat{h}_g^{j+1}}{dt} \]
\[ + (1 - \alpha) M^j \cdot \frac{d\hat{h}_g^j}{dt} = \alpha F^{j+1} + (1 - \alpha) F^j \] (3.43)

It must be noted that in saturated unconfined aquifer flow, the mass matrix, \( M \), is a constant matrix which is not a function of hydraulic head and takes the same values for all time steps. Therefore, the above formulation can be simplified as:

\[ \alpha S^{j+1} \cdot \hat{h}_g^{j+1} + (1 - \alpha) S^j \cdot \hat{h}_g^j + M \cdot \left( \alpha \frac{d\hat{h}_g^{j+1}}{dt} + (1 - \alpha) \frac{d\hat{h}_g^j}{dt} \right) = \alpha F^{j+1} + (1 - \alpha) F^j \] (3.44)

It is now possible to substitute for the weighted averaged derivative terms given in equation (3.40) for the term in the parenthesis to obtain:

\[ \alpha S^{j+1} \cdot \hat{h}_g^{j+1} + (1 - \alpha) S^j \cdot \hat{h}_g^j + M \cdot \left( \frac{\hat{h}_g^{j+1} - \hat{h}_g^j}{\Delta t} \right) = \alpha F^{j+1} + (1 - \alpha) F^j \] (3.45)

After rearrangement, the equation takes the following final from:

\[ \left( \alpha S^{j+1} + \frac{M}{\Delta t} \right) \cdot \hat{h}_g^{j+1} = \alpha F^{j+1} + (1 - \alpha) F^j - \left( (1 - \alpha) S^j - \frac{M}{\Delta t} \right) \cdot \hat{h}_g^j \] (3.46)

From equation (3.46), one can obtain different time integration schemes depending on the value of the time weighing parameter. Even though infinitely many values of the weighing parameter are possible, several of these are particularly important and have significant properties. With \( \alpha = 0 \), the equation becomes an explicit scheme and it does not require the solution of any system of equations in order to advance the solution across time. However, explicit schemes often encounter numerical instabilities if the time step is taken too large. When \( \alpha = 0.5 \), the scheme becomes the so-called Crank-Nicholson method, which implements a central-difference approximation between two time lines. It is known that this choice of the time weighing factor corresponds to the optimal sampling of the first temporal derivative over the time step. If the data of the problem have sufficient continuity, this scheme exhibits its optimal accuracy properties and results in a very efficient method for handling the time-dependence of the transient problem. Unfortunately, presence of any discontinuity in the data might lead to spurious oscillations of the computed solution. If \( \alpha = 1 \), the scheme becomes a fully-implicit scheme and resists the development of solution oscillations better than any other one-step method. Therefore, it is commonly used for most difficult problems. However, it should be noted that this scheme is not fully accurate or especially efficient but it will dampen spurious high-frequency effects more strongly than
the other schemes. Based on this discussion, a time-weighing parameter of 0.5 is selected to be used in this study.

The governing equation of unconfined aquifer is non-linear since the saturated thickness is a function of hydraulic head. Therefore, the discretized equations are to be solved in an iterative manner. Common non-linear solution techniques such as Newton-Raphson method or successive substitution (Picard iteration) method can be applied in this solution. Although the Newton-Raphson method is faster in convergence, it requires the computation of partial derivatives that is rather costly in finite element framework. Hence, the relatively simple Picard iteration technique is applied in the solution of the groundwater flow model. The Picard method is a very simple technique and is based on successively substituting the latest values of the hydraulic head to compute new values until sufficient convergence is achieved. When Picard method is applied, the discretized groundwater flow equation can be written as:

\[
\left( \alpha S^{j+1,k} + \frac{M}{\Delta t} \right) \cdot \hat{h}_g^{j+1,k+1} = \alpha F^{j+1,k} + (1 - \alpha)F^j - \left( (1 - \alpha)S^j - \frac{M}{\Delta t} \right) \cdot \hat{h}_g^j
\]

where superscripts \( k \) and \( k+1 \) represent previous and current iteration values of hydraulic head at the unknown time level. For all iterations, most recent values of the hydraulic heads are used to obtain an improved estimate of the heads at the unknown time level according to the following formula:

\[
\hat{h}_g^{j+1,k+1} = \gamma \hat{h}_g^{j+1,k+1} + (1 - \gamma)\hat{h}_g^{j+1,k}
\]

where \( \gamma \) is an iteration-dependent under-relaxation coefficient (or a damping parameter) taking values between 0 and 1. The left hand-side value at \((k+1)\)th iteration represents the improved estimate to be used in next iteration. For very non-linear problems, head change in iterations might be large enough to cause the solution to oscillate. In such cases, a damping parameter can be used to restrict the head change from one iteration cycle to the next (Huyakorn et al., 1986). In each iteration cycle, the value of damping parameter is computed according to the following procedure:

\[
\gamma = \begin{cases} 
\frac{3 + s}{3 + |s|} & s \geq -1 \\
\frac{1}{2|s|} & s < -1 
\end{cases}
\]

where \( s \) is a scale parameter evaluated according to the following rule:
\[
S = \begin{cases} 
1 & k = 1 \\
\frac{\varepsilon_{k+1}}{\gamma_{\text{old}} \varepsilon_k} & k > 1
\end{cases}
\] (3.50)

where \( \varepsilon_{k+1} \) and \( \varepsilon_k \) represent the hydraulic head change for iteration \( k+1 \) and \( k \), respectively, that is largest in absolute value and \( \gamma_{\text{old}} \) is the value of damping parameter at the previous iteration.

### 3.2.5. Model Testing

As there are no documented analytical solutions for the unsteady groundwater flow in two dimensions, the proposed model is tested against two different sets of analytical solutions developed within a one dimensional framework. The first analytical solution is based on the simulation of a canal-aquifer system as shown in Figure 3.8. The water level in the canal as well as the aquifer is initially horizontal at a level \( h_{g1} \). The water level in the canal is raised instantaneously to an elevation \( h_{g2} \) above the datum line and maintained constant thereafter creating an increase in the aquifer head, \( h_g \). The one dimensional mathematical model of this bank storage flow problem is given as:

\[
S_y \frac{\partial h_g}{\partial t} = K \frac{\partial}{\partial x} \left( h_g \frac{\partial h_g}{\partial x} \right)
\] (3.51)

with the following initial and boundary conditions:

\[
h_g(x, 0) = h_{g1} \\
h_g(0, t) = h_{g2} \\
h_g(\infty, t) = h_{g1}
\] (3.52)

where it is assumed that the aquifer has uniform hydraulic conductivity. The model assumes that the aquifer is homogeneous and isotropic and rests on a horizontal impervious base. In addition, the sediment layer between the canal and aquifer has the same conductivity as the aquifer.

Following suitable linearizations, the governing equation could be written in the following form:

\[
\frac{\partial h_g^2}{\partial t} = \overline{\sigma} \frac{\partial^2 h_g^2}{\partial x^2}
\] (3.53)

where the parameter \( \overline{\sigma} \) is given as:
\[ \vec{v} = \frac{K \bar{h}_g}{S_y} \]  

(3.54)

with \( \bar{h}_g \) is a weighted average of the depth of saturation during the period of flow. The analytical solution to this model is given by Marino and Luthin (1982):

\[
h_g^2(x,t) = h_{g,0}^2 + \left( h_{g,t}^2 - h_{g,0}^2 \right) \text{erfc} \left( \frac{x}{\sqrt{4\mu t}} \right)
\]

(3.55)

where \text{erfc} is the complimentary error function. To test the model’s capability against this analytical solution, a hypothetical aquifer-canal system is constructed in which flow is assumed to be one directional. Linear square elements of 5m side length are assembled to create an unconfined aquifer of 100m long such that the assumption of infinite aquifer is satisfied during the 10-hr simulation period. A uniform hydraulic conductivity field of 0.001m/s is used in the simulations. The initial water level in the canal and in the aquifer is taken to be 5m. The water level in the aquifer is instantaneously increased to 7m and kept constant at this level throughout the simulation. The groundwater movement in the aquifer is then simulated with the proposed model. The comparison of analytically computed and numerically simulated groundwater heads are given in Figure 3.9. As seen from the figure, the numerically simulated values are almost identical to the analytically calculated groundwater heads. It is also important to note that the level of fit does not deteriorate with time which is an important issue in time-dependent solutions.

Figure 3.8. Rise of water level in a semi-infinite unconfined aquifer
Figure 3.9. Comparison of simulated hydraulic heads and analytical solution of canal-aquifer system
In the second test, the model is verified with the analytical solution of Marino (1967) that describes the growth and decay of groundwater ridges due to vertical percolation (i.e., infiltration). Figure 3.10 shows a cross-section of an unconfined aquifer assumed to be infinite in areal extent and receiving uniform vertical percolation. The rate of percolation is maintained by a spreading area in the form of an infinitely long strip located above the main unconfined aquifer. After sufficient time, a groundwater ridge develops and initiates groundwater flow. The mathematical model for this flow system is written as in two separate zones. Zone 1 is defined as the region where the infiltration occurs. Zone 2, on the other hand, starts from the edge of Zone 1 extending throughout the aquifer and does not receive infiltration. The mathematical model of this problem is defined by the following boundary value problem (Marino, 1967):

\[
\begin{align*}
\text{ZONE } & 1: \\
& \frac{1}{\nu} \frac{\partial h_{x1}}{\partial t} = \frac{\partial^2 h_{x1}}{\partial x^2} + Af(t) \\
& f(t) = \begin{cases} 
1 & 0 < t \leq t_i \\
0 & t > t_i 
\end{cases} \\
\text{ZONE } & 2: \\
& \frac{1}{\nu} \frac{\partial h_{x2}}{\partial t} = \frac{\partial^2 h_{x2}}{\partial x^2}
\end{align*}
\]

where \( t_i \) is the time period during which vertical percolation or infiltration, \( I \), occurs and the parameter \( A \) is equal to \( 2I/K \). The following initial and boundary conditions are used to supplement the equation:

\[
\begin{align*}
\text{ZONE } & 1: \\
& h_{x1}(x,0) = h_{x,x,0} \\
& Kh_{x1} \frac{\partial h_{x1}}{\partial x} \bigg|_{x=0,t>0} = 0 \\
\text{ZONE } & 2: \\
& h_{x2}(x,0) = h_{x,x,0} \\
& h_{x2}(\infty,t) = h_{x,x,0}
\end{align*}
\]

At the internal boundary between zones 1 and 2 (i.e., \( x=L \)), it is possible to write the continuity of mass fluxes and equality of hydraulic heads such that:

\[
\begin{align*}
& h_{x1}(L,t) = h_{x2}(L,t) \\
& Kh_{x1} \frac{\partial h_{x1}}{\partial x} \bigg|_{x=L,t>0} = Kh_{x2} \frac{\partial h_{x2}}{\partial x} \bigg|_{x=L,t>0}
\end{align*}
\]

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Figure 3.10. Schematic of growth and decay of groundwater ridges
Marino (1967) developed the analytical solution for this problem by applying Laplace transform with respect to $t$ and presented the results both for the period when infiltration occurs and for the period after it ceases. During the infiltration period $0 < t \leq t_i$, the analytical solution is written as:

$$h_{g1}^2 = h_{g,0}^2 + \frac{2I\bar{\Omega}t}{K} - \frac{I\bar{\Omega}t}{K} \left[ 4i^2\text{erfc} \left( \frac{L-x}{\sqrt{4\bar{\Omega}t}} \right) + 4i^2\text{erfc} \left( \frac{L+x}{\sqrt{4\bar{\Omega}t}} \right) \right]$$

$$h_{g2}^2 = h_{g,0}^2 + \frac{I\bar{\Omega}t}{K} \left[ 4i^2\text{erfc} \left( \frac{x-L}{\sqrt{4\bar{\Omega}t}} \right) - 4i^2\text{erfc} \left( \frac{x+L}{\sqrt{4\bar{\Omega}t}} \right) \right]$$

(3.59)

Similarly, for $t > t_i$, the analytical solution becomes:

$$h_{g1}^2 = h_{g,0}^2 + \frac{2I\bar{\Omega}t}{K} - \frac{I\bar{\Omega}t}{K} \left[ 4i^2\text{erfc} \left( \frac{L-x}{\sqrt{4\bar{\Omega}t}} \right) + 4i^2\text{erfc} \left( \frac{L+x}{\sqrt{4\bar{\Omega}t}} \right) \right]$$

$$- \frac{2I\bar{\Omega}t'}{K} - \frac{I\bar{\Omega}t'}{K} \left[ 4i^2\text{erfc} \left( \frac{L-x}{\sqrt{4\bar{\Omega}t}} \right) + 4i^2\text{erfc} \left( \frac{L+x}{\sqrt{4\bar{\Omega}t}} \right) \right]$$

$$h_{g2}^2 = h_{g,0}^2 + \frac{I\bar{\Omega}t}{K} \left[ 4i^2\text{erfc} \left( \frac{x-L}{\sqrt{4\bar{\Omega}t}} \right) - 4i^2\text{erfc} \left( \frac{x+L}{\sqrt{4\bar{\Omega}t}} \right) \right]$$

$$- \frac{I\bar{\Omega}t}{K} \left[ 4i^2\text{erfc} \left( \frac{x-L}{\sqrt{4\bar{\Omega}t'}} \right) - 4i^2\text{erfc} \left( \frac{x+L}{\sqrt{4\bar{\Omega}t'}} \right) \right]$$

(3.60)

where $t' = t - t_i$ is the time since the cessation of vertical percolation and $4i^2\text{erfc}(y)$ is the second repeated integral of the error function of the argument $y$ (Carslaw and Jaeger, 1959).

The proposed groundwater flow model is tested against the analytical solution of Marino (1967) given in equation (3.60). In his paper, Marino compared his analytical solution with a laboratory scale experiment. His experimental setup included a 100cm long plume filled with a soil that has a conductivity value of 0.42cm/s. A 23.8cm long apparatus provides the uniform infiltration rate of 5.6E-2cm/s over the aquifer. The experiment is conducted with an initial groundwater head of 11.3cm. In his study, Marino (1967) provides a good fit between measured and analytically calculated hydraulic head values. In this study, a numerical model is constructed to duplicate the aquifer conditions of Marino (1967) and the results from his analytical solution and laboratory experiments are compared with the numerically computed values. In the numerical model, the spatial discretization of the experimental aquifer is done with square finite elements that have a side length of 5cm. The temporal discretization is done with 10sec to cover a total simulation period of 660sec. Marino (1967) has used the observation points of his experimental setup to compute the
values of the analytical solution and presented his analytical solution at these discrete points. Following Marino’s approach, the analytical solution values are given discretely and the numerical solution is presented as a continuous line for accurate comparison of the analytically computed and numerically simulated groundwater heads (Figure 3.11). When the figure is analyzed, one can see that a fairly close fit is obtained between the numerically computed results and Marino’s analytical and experimental results. Although the deviation is fairly small (i.e., less than 10%), the numerically simulated hydraulic head values start to deviate from the analytical solution as a function of time. It is interesting to note that the level of fit with the observed values is much better then the level of fit with the analytical solution.

3.3. Two Dimensional Overland Flow Model

3.3.1. Governing Equations

The governing equation of overland flow model is obtained by introducing the non-inertia wave-approximation to the general continuity and momentum equations of the two-dimensional shallow water flow. The non-inertia or diffusion wave approximation is suitable for areas with mild topography where downstream backwater effect is important but accelerations are relatively small. Numerous researchers have chosen the non-inertia wave approximation to simulate shallow water hydrodynamics in order to reduce computational efforts without sacrificing accuracy (Hromadka II and Yen, 1986; Feng and Molz, 1997; Morita and Yen, 2002). For an anisotropic, non-homogeneous ground surface with principle diffusion directions matching the coordinate directions, the governing equation of overland flow is written as:

\[ \frac{\partial h_o}{\partial t} - \frac{\partial}{\partial x} \left( K_{o_x} \frac{\partial h_o}{\partial x} \right) - \frac{\partial}{\partial y} \left( K_{o_y} \frac{\partial h_o}{\partial y} \right) - R + I = 0 \]  

(3.61)

where \( x \) and \( y \) are the spatial coordinates in the horizontal domain, \( t \) is the temporal coordinate, \( h_o \) is the water surface elevation of overland flow, \( R \) is the rainfall rate, \( I \) is the infiltration rate, and \( K_{o_x} \) and \( K_{o_y} \) are the diffusion coefficients in \( x \)- and \( y \)- directions of flow given by:

\[ K_{oi} = \frac{1}{(n_o)_i^2} \left[ \left( \frac{\partial h_o}{\partial x} \right)^2 \frac{1}{(n_o)_x^4} + \left( \frac{\partial h_o}{\partial y} \right)^2 \frac{1}{(n_o)_y^4} \right]^{1/4} \]

\[ i = x, y \]  

(3.62)

where \( z_g \) is the ground surface elevation and \( n_o \) is the Manning’s roughness coefficient for overland flow.
Figure 3.11. Comparison of simulated, observed and analytical hydraulic heads
It is important to note that friction factors for overland flow in natural areas are difficult to conceptualize from pure theory alone. Except for flow over man-made surfaces such as asphalt or concrete, overland flow is usually a very complex hydraulic and geometric phenomenon. Ideally, different friction factors must be used to cover different flow regimes, and the dynamic effects of rainfall impact, channelization of flow, obstacles such as litter, crop ridges and rocks and erosion must all be considered during the formulation of a total friction coefficient. On the other hand, from a practical engineering standpoint, an “effective” coefficient of friction is adequate for applied cases of simulating an overland flow hydrograph or computing travel times.

Overland flow typically occurs in wide thin films with very small depths (i.e., less than a couple of centimeters) and relatively small velocities (i.e., less than 0.1 m/s). These typical values result in relatively small Reynolds numbers when compared to open channel flow. The flow is typically considered to be laminar if only Reynolds number is considered as a factor. However, the hydraulics of overland flow is much more complicated and numerous additional factors are to be addressed when quantifying this complex event such as the added turbulence due to rainfall impact, vegetation and channelized flow as well as the non-fixed bed phenomena due erosion (Dingman, 1994). In this regard, a general consensus has been achieved among hydraulics experts that the overland flow covers both laminar and turbulent flows and is considered to change from laminar to turbulent and back to laminar through the rise and recession of a hydrograph (Engman, 1986).

The most theoretically sound friction formulae that can cover the entire flow spectrum is the Darcy-Weisbach relationship. This relationship was originally developed for pipe flow and found wide applicability in pipe flow hydraulics. It included relative roughness and Reynolds number as two parameters required to find the roughness coefficient. However, the difficulty in obtaining an accurate roughness parameter helped other resistance expressions, such as the Manning and Chezy formulae, find wider applicability especially in open channel flow where flow is mostly characterized in the turbulent regime. Consequently, a wide collection of Manning and Chezy resistance coefficients accumulated in time, which further promoted their use in simulation models. Nevertheless, Darcy-Weisbach relation still remained the method of choice when the flow is out of the turbulent regime and/or when there is sufficient data from the field.

Considering the scale of modeling effort and the accuracy of the available data, it is practically wise to use a single value for the resistance coefficient that basically assumes that the overland flow is turbulent. In this context, the effect of rainfall impact, vegetation, channelized flow and all other possible factors are lumped in an effective friction coefficient. This approximation is clearly justifiable from an engineering perspective for a distributed hydrological model of watershed scale. From this token, it is possible to use Manning resistance factor and equation to formulate the friction slope in non-inertia wave equations. Essentially, Manning roughness coefficient not only includes all the uncertainty in terms of process theory and data limitations but also covers our ignorance in terms of the effects of unsteadiness and non-uniformity of flow.
3.3.2. Initial Conditions

In the overland flow model, the initial conditions are given by specifying the water surface elevation at all points in the two-dimensional domain. In representing an initially dry overland surface, a very thin water film is assumed before the flow is initiated such that (Akan and Yen, 1981a):

\[ h_o(x, y, 0) = h_{o0}(x, y) \]  \hspace{1cm} (3.63)

This artificial assignment of an initial water depth facilitates the numerical solution procedure. As a rule of thumb, \( h_{o0} \) can be taken to be less than or equal to 0.1 mm to alleviate any possible numerical problems that might arise otherwise.

3.3.3. Boundary Conditions

Although overland flow is basically a source/sink driven flow mechanism, two different types of boundary conditions are still specified along different external boundaries of overland flow domain. Type-1 or specified head boundary conditions are generally used to model boundaries with known water surface elevation and are given as:

\[ h_o(x, y, t) = h_{oD}(x, y, t) \]  \hspace{1cm} (3.64)

where \( h_{oD} \) is the known water surface elevation. Type-2 or specified flux boundary conditions are used to model boundaries with known flux values. It is also known as a Neumann boundary condition and is given as:

\[ q_N(x, y, t) = -\mathbf{n} \cdot (K_o \cdot \nabla h_o) = -\mathbf{n} \cdot (\mathbf{V} (h_o - z_g)) \]  \hspace{1cm} (3.65)

where \( q_N \) is the known flux value and \( \mathbf{n} \) is the unit normal to the boundary. Although it is theoretically possible to define a head-dependent boundary condition for overland flow, it is generally not implement for the sake of simplicity since it is practically very difficult to keep track of changing stages over the land in a precipitation event.

3.3.4. Numerical Solution Scheme

In general, the finite difference and finite element methods are widely applied in overland flow modeling (Akan and Yen, 1981b; Hromadka and Yen, 1986; Akanbi and Katapodes, 1988; Zhang and Cundy, 1989; Motha and Wigham, 1995; Feng and Molz, 1997; Lal, 1998; Dutta et al., 2000; Gandolfi and Savi, 2000; Morita and Yen, 2002; Bradford and Sanders, 2002). For watershed-scale applications where topography is highly variable, finite element method is proven to be more powerful compared to finite difference method due to the flexibility it offers in simulating land surfaces with spatially variable land use/cover patterns and irregular boundaries. Hence, the Galerkin finite element method
based on the method of weighted residuals is used in this study to solve the overland flow equation.

The overland flow surface is discretized with two-dimensional quadrilateral finite elements such that the material properties of the domain (i.e., the roughness coefficient) are retained in individual elements. Following the idealization of domain and selection of the interpolating functions, an appropriate weak form of the problem is developed as shown in Gunduz (2004). The resulting finite element matrix equation obtained by applying the Galerkin procedure is given as:

$$\mathbf{S} \cdot \mathbf{\hat{h}}_o + \mathbf{M} \cdot \frac{d \mathbf{\hat{h}}_o}{dt} = \mathbf{F}$$  \hspace{1cm} (3.66)

where \(\mathbf{S}\), \(\mathbf{M}\) and \(\mathbf{F}\) stand for global stiffness matrix, global mass matrix and global load vector, respectively, and \(\mathbf{\hat{h}}_o\) is the overland flow stage vector. The explicit formulas of element matrices and vectors are also derived in Gunduz (2004). As these element integrals are generally complex and cannot be integrated analytically, a two-dimensional Gaussian quadrature technique is implemented to numerically integrate the integrals. When the same procedure implemented in the derivation of the groundwater flow equation is followed, one would obtain the final form of the discretized equation as:

$$\left(\alpha \mathbf{S}^{j+1} + \frac{\mathbf{M}}{\Delta t}\right) \cdot \mathbf{\hat{h}}_o^{j+1} = \alpha \mathbf{F}^{j+1} + (1 - \alpha) \mathbf{F}^j - \left(1 - \alpha\right) \mathbf{S}^j - \frac{\mathbf{M}}{\Delta t}\right) \cdot \mathbf{\hat{h}}_o^j$$  \hspace{1cm} (3.67)

Although different time integration schemes are now possible, a Crank-Nicholson scheme with \(\alpha=0.5\) is used in this study. This scheme provides the ideal approximation between two time lines.

The overland flow equation is a highly non-linear equation since the diffusion coefficients are non-linear functions of the dependent variable (i.e., stage). To handle this non-linearity, the Picard iteration is used in this study such that the latest values of the stage are successively substituted to compute new values until sufficient convergence is achieved. When Picard method is applied, the discretized overland flow equation can be written as:

$$\left(\alpha \mathbf{S}^{j+1,k} + \frac{\mathbf{M}}{\Delta t}\right) \cdot \mathbf{\hat{h}}_o^{j+1,k+1} = \alpha \mathbf{F}^{j+1,k} + (1 - \alpha) \mathbf{F}^j - \left(1 - \alpha\right) \mathbf{S}^j - \frac{\mathbf{M}}{\Delta t}\right) \cdot \mathbf{\hat{h}}_o^j$$  \hspace{1cm} (3.68)

where superscripts \(k\) and \(k+1\) represent previous and current iteration values of stage at the unknown time level.
3.3.5. Model Testing

The overland flow model is probably the most difficult of the four major flow pathways discussed in this study. Even for a single event simulation, the model contains difficulties in defining the time dependent spatial extent of the flow phenomena as it changes continuously according to the flow characteristics and the spatially variability of the precipitation event. Although there are no analytical solutions to the two dimensional non-inertia wave form of the model, it is possible to write a simple analytical solution for the simplified kinematic wave form of the model in one-dimensional setup (Stephenson and Meadows, 1986). The proposed model is tested against this analytical solution and the data collected from a test plot by Izzard (1946).

The kinematic wave model neglects not only the local and convective acceleration terms but also the pressure term in the momentum balance equation of the original St. Venant equations. It inherently assumes that the bed slope is equal to the friction slope in the channel. The kinematic wave model does not allow upstream migration of disturbances so is not suitable to systems with backwater phenomenon. It is, however, found to be suitable for modeling overland flow in some upland watersheds as well as modeling channel flow in small streams with moderate to high bed slopes (Stephenson and Meadows, 1986).

The kinematic wave model is written by the continuity equation and the simplified momentum equation by using the Manning’s expression to define the velocity in the channel such that:

\[
\frac{\partial d}{\partial t} + m \alpha_k (d)^{m-1} \frac{\partial d}{\partial x} = R - I
\]

(3.69)

where \(d\) is the water depth in the channel, \(m\) is a constant that is equal to 5/3 and \(\alpha_k\) is a constant that is a function of surface roughness and bed slope written as:

\[
\alpha_k = \frac{\sqrt{S_b}}{n}
\]

(3.70)

According to Stephenson and Meadows (1986), the analytical solution to the kinematic wave model in response to a uniform rainfall event with no infiltration is given as:

\[
q = \begin{cases} 
\alpha (Rt)^m & \text{for} \quad 0 \leq t \leq t_c \\
\alpha (Rt_c)^m & \text{for} \quad t_c \leq t \leq t_r \\
RL - Rm\alpha^{1/m}(m-1)/m (t - t_r) & \text{for} \quad t_r \leq t \leq t_f
\end{cases}
\]

(3.71)

where \(q\) is the discharge per unit width, \(t_c\) is the time of concentration, \(t_r\) is the duration of the rainfall event and \(t_f\) is the total simulation time. The time of concentration is defined as
the time at which the entire watershed starts to contribute to the outflow and is given by the expression:

\[ t_c = \left( \frac{L}{\alpha R^{m-1}} \right)^{\frac{1}{m}} \]  

(3.72)

The proposed model is verified using the above model on a hypothetical test bed with a length of 100 m and a bed slope of 0.001 m/m. The Manning’s roughness coefficient is taken to be 0.02. A constant rainfall rate of 2.78E-6 m/s is applied for 8000 sec over the entire test bed and the model is simulated for a total of 15000 sec. The analytically computed and numerically simulated discharge per unit width values obtained at the outlet of the bed is shown in Figure 3.12. As seen from the figure, the proposed model gives a very close fit to the analytical solution. Only just before the time of concentration, the proposed model creates a much smoother transition to the peak value whereas as the analytical solution produces a sharper pass.

In the second example, the proposed model is tested against the experimental work of Izzard (1946). Izzard analyzed the overland flow from paved and turf surfaces and performed a series of tests which he called as ‘runs’. The Run-136 of Izzard (1946) is used to test the model. The experimental plot in his run was a 72 m long plume with 0.01 ft/ft bed slope. The plume was an asphalt plane with a Manning’s roughness value of 0.024. In his Run-136, Izzard used a two stage rainfall event with both stages having a magnitude of 3.56 inch/hr. The proposed model is run with the same data and the results are compared in Figure 3.13.

As seen from this figure, the proposed model accurately predicts the peak discharge, time to peak and rising and falling limbs of the hydrograph. However, it shows slight deviations from Izzard’s experimental data during the transition to the peak value and during the minimum flow period between the two rainfall steps. Overall, the level of prediction by the model is considered to be satisfactory.

### 3.4. One Dimensional Unsaturated Groundwater Flow

#### 3.4.1. Governing Equations

The movement of soil moisture in the variably-saturated unsaturated zone is modeled by using the Richards’ equation which is supplemented by constitutive relations to describe the relationship among fluid pressure, water saturation and unsaturated hydraulic conductivity. In an anisotropic, non-homogeneous media, the mixed-form of the equation with both the water content and the pressure head as the dependent variables is given as (Miller et al., 1998):
Figure 3.12. Comparison of simulated unit discharge and analytical solution of overland flow
where $z$ is the spatial coordinates in the vertical domain, $t$ is the temporal coordinate, $S_w$ is the degree of saturation, $S_s$ is the specific storage coefficient, $\Psi$ is the capillary pressure head, $\theta$ is the volumetric water content and $K_u$ is the unsaturated hydraulic conductivity in vertical direction. To complete the mathematical representation of moisture movement in the unsaturated zone, soil-water retention and hydraulic conductivity relationships that relate the capillary pressure head to soil moisture and hydraulic conductivity must also be provided such as the ones shown in Figure 3.14.

Although the relationships developed by Brooks and Corey (1964), Campbell (1974), Mualem (1976), Clapp and Hornberger (1978) and van Genuchten (1980) are used extensively in the solution of the Richards equation, detailed analysis reveals that only the expressions of van Genuchten (1980) would describe the entire pressure spectrum including the saturated portion above the bubbling pressure. Therefore, the $\theta-\psi$ and $K-\psi$ relations of van Genuchten (1980) are used in this study:
\[ S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[ 1 + \left( \alpha_s |\psi| \right)^{n_v} \right]^{-m_v} \]  

(3.74)

\[
K_s (\psi) = \left( K_{gs} \right) z \frac{\left\{1 - \left( \alpha_r |\psi| \right)^{n_v-1} \left[ 1 + \left( \alpha_s |\psi| \right)^{n_v} \right]^{-m_v} \right\}^2}{\left[ 1 + \left( \alpha_s |\psi| \right)^{n_v} \right]^{-m_v/2}}
\]  

(3.75)

where \( S_e \) is the effective saturation, \( \theta_r \) is the residual water content, \( \theta_s \) is the saturated water content, \( K_g \) is the saturated hydraulic conductivity, \( n_v \) and \( m_v \) are constants that depend on soil type and \( m_v \) is equal to \( \left( 1 - 1/n_v \right) \).

3.4.2. Initial Conditions

The initial conditions provide the values of capillary pressure head and/or soil moisture at all points in the vertical domain at the beginning of the simulation. Therefore, if \( z_g \) and \( z_{wt} \) represent the elevations of the ground surface and the water table, respectively, the initial conditions can be written as a function of pressure head or water content such that:

\[
\psi (z, 0) = \psi_0 (z) \quad \text{for} \quad z_{wt} \leq z \leq z_g \]  

(3.76)

\[
\theta (z, 0) = \theta_0 (z) \quad \text{for} \quad z_{wt} \leq z \leq z_g \]  

(3.77)

where \( \psi_0 \) is the initial capillary pressure head and \( \theta_0 \) is the initial water content within the domain.

![Figure 3.14. Typical soil water retention curves for (a) hydraulic conductivity and (b) water content in unsaturated porous media](image_url)
3.4.3. Boundary Conditions

The boundary conditions are defined at the top and bottom of the domain. In this study, the top boundary condition is taken as the soil surface and the bottom boundary condition is selected to be the groundwater table. At the ground surface, the boundary condition switches between specified head and specified flux depending on the conditions of the overland flow (Gunduz and Aral, 2003c):

\[
\psi (z_g, t) = \psi_g (t)
\]
\[-K(\psi) \frac{\partial (\psi + z)}{\partial z} = q_g (t)
\]

(3.78)

where \(\psi_g\) is the positive overland flow depth over the ground surface and \(q_g\) is the infiltration/exfiltration flux at the surface. At the water table, on the other hand, a zero pressure head specified boundary condition is defined at all times:

\[
\psi (z_w, t) = 0
\]

(3.79)

3.4.4. Numerical Solution Scheme

In numerical solution of the Richards’ equation, the spatial discretization is commonly performed by (i) finite difference and (ii) finite element methods (Celia et al., 1990; Gottardi and Venutelli, 1993a; Rathfelder and Abriola, 1994; Pan et al., 1996; Miller et al., 1998; Van Dam and Feddes, 2000; Zhang et al., 2002). Both methods are commonly used in the literature and neither method really favors the other. Regardless of the spatial discretization method used, the time approximation commonly involves a fully implicit approximation of the time derivative.

The Picard iteration, Modified Picard iteration or Newton-Raphson iteration are frequently used to resolve the nonlinearities in the Richards’ equation. While the first two converge linearly, the Newton iteration converges quadratically in the vicinity of the solution, which might lead to more efficient solutions depending on the type of nonlinearity. Paniconi et al. (1991) and by Miller et al. (1998) studied the numerical properties of iterative methods and found out that both the linearly-converging and the quadratically-converging methods provide similar convergence rates especially for strong nonlinear situations with linearly-converging methods requiring much less computational power.

In this study, the numerical solution of the Richards’ equation is done with a standard central difference control volume finite difference approximation to discretize the spatial derivatives and a first-order backward finite difference approximation to discretize the time derivatives. The modified Picard iteration of Celia et al. (1990) is then implemented to solve for the nonlinearity. The details of the numerical solution method are given in Gunduz (2004). The discretized form of equation (3.73) is the core of the unsaturated zone
flow model. This equation is written for each intermediate node of the domain, and supplemented by the discretized forms of the boundary condition equations at the top and bottom of the domain. For each intermediate node, the final form of the discretized Richards’ equation is written as:

\[
(S_u S_v)_{i,j,k}^{j+1,k} \left[ \frac{\psi_{i,j+1,k}^{j+1,k} - \psi_{i,j}^{j}}{\Delta t} \right] + \left[ \theta_i^{j+1,k} + C_i^{j+1,k} \left( \psi_{i,j+1,k+1}^{j+1,k} - \psi_{i,j+1,k}^{j} \right) - \theta_i^{j} \right]
\]

\[
- \frac{1}{\Delta z_i} \left[ (K_u)_{i+1/2}^{j+1,k} \left( \frac{\psi_{i+1,j+1,k+1}^{j+1,k} - \psi_{i+1,j+1,k}^{j}}{\Delta z_{i+1/2}} + 1 \right) - (K_u)_{i-1/2}^{j+1,k} \left( \frac{\psi_{i-1,j+1,k+1}^{j+1,k} - \psi_{i-1,j+1,k}^{j}}{\Delta z_{i-1/2}} + 1 \right) \right] = 0 \quad (3.80)
\]

where subscripts \(i, j\) and \(k\) represent the spatial, temporal and iteration indices, respectively. The three pressure heads at nodal points \(i-1, i\) and \(i+1\) at the unknown iteration level are the unknowns in the above equation. When written for all intermediate nodes, one would obtain a system of \(N-2\) nonlinear equations with \(N\) unknowns. Upon including the two equations for the top and bottom boundary conditions, the system could be written as:

\[
[\alpha A^{j+1,k} + (1 - \alpha) A^j].x^{j+1,k+1} = \alpha f^{j+1,k} + (1 - \alpha)f^j \quad (3.81)
\]

where \(A\) is the coefficient matrix, \(x\) is the unknown vector and \(f\) is the known right hand side vector. This matrix equation is then solved by a suitable matrix solver. Due to three-diagonal structure of the coefficient matrix, the efficient Thomas algorithm provides the best solution for this system.

### 3.4.5. Model Testing

The one-dimensional unsaturated groundwater flow equation is a difficult non-linear partial differential equation due to the strong dependency of both the hydraulic conductivity and the water content on the capillary pressure. The empirical soil-water retention and conductivity relationships such as the van Genuchten model are the source of this non-linearity. In this regard, there are no known analytical solutions to the one-dimensional Richards’ equation with realistic soil-water relationships. Nevertheless, numerous researchers including Philip (1969), Warrick (1975), Sander et al. (1988), Warrick et al. (1990), Srivastava and Yeh (1991), Warrick et al. (1991), Barry et al. (1993), Tracy (1995), Marinelli and Durnford (1998), Hogarth and Parlange (2000) and Chen et al. (2003) have developed various forms of exact solutions under fairly strict limitations. In all of these studies, the problematic soil-water relations are simplified and linearized by using various transformations and/or trouble-free linear functions. Therefore, it is believed that these solutions have very limited applicability in testing a practical model based on strongly non-linear soil-water relations such as the one of van Genuchten. In addition, these exact solutions are almost always extremely complicated, and require numerical methods which sometimes make them more labor intensive than the original numerical model used to solve the governing partial differential equation.
Considering the factors discussed above, the proposed unsaturated zone flow model is tested against a well-documented and verified commercial software such as HYDRUS-1D of Simunek et al. (1998) as well as the results from a benchmark paper by Celia et al. (1990). Three different tests are simulated with both the HYDRUS model and the proposed model to test the proposed model’s capabilities with different soil types and soil hydraulic parameters as well as different boundary conditions. The first test is called the Skagg’s column infiltration test and is intended to simulate infiltration into a 60cm column having -150cm initial pressure head. Constant pressure head values of -150cm and -1cm are applied at the bottom and top of the column as constant head boundary conditions, respectively. The hydraulic parameters of the soil are given in Table 3.1. The moisture is allowed to migrate along the column for 2.5hrs and the advancing front is tracked within the column. The pressure head distribution is simulated with both HYDRUS and the proposed model and the results are shown in Figure 3.15 for various instances in time.

Table 3.1. Soil Hydraulic Parameters of Test Cases

<table>
<thead>
<tr>
<th></th>
<th>$\theta_s$ (-)</th>
<th>$\theta_r$ (-)</th>
<th>$\alpha$ (cm$^{-1}$)</th>
<th>$n$ (-)</th>
<th>$K_s$ (cm/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEST 1</td>
<td>0.3500</td>
<td>0.020</td>
<td>0.0410</td>
<td>1.964</td>
<td>2.5992000</td>
</tr>
<tr>
<td>TEST 2</td>
<td>0.4300</td>
<td>0.078</td>
<td>0.0360</td>
<td>1.560</td>
<td>1.0400004</td>
</tr>
<tr>
<td>TEST 3</td>
<td>0.3308</td>
<td>0.000</td>
<td>0.0143</td>
<td>1.506</td>
<td>25.000000</td>
</tr>
</tbody>
</table>

The first test case demonstrates the capabilities of the proposed model in simulating the characteristics of infiltration into a moderately dry soil. It can be seen from Figure 3.15 that the model performs extremely well in simulating the vertical movement of soil moisture in vertical direction. It is clearly seen that the results obtained from the proposed model are indistinguishable from the HYDRUS model. Moreover, the downward movement of the wetting front is accurately captured by the proposed model both in space and in time.

The second test is a demonstration of simulating an exfiltration condition where moisture movement is opposite to the gravitational acceleration. It is a condition in which the vertical drainage is overcome by the strong pressure gradient between the surface and the bottom boundary conditions. A 7.6cm column is discretized in a non-uniform fashion such that the highly variable pressure head conditions at the bottom boundary could be captured accurately. A strongly dry initial condition (i.e., -750cm pressure head) is used to start the simulation. The bottom boundary condition is selected to be a -1cm constant head that is used to drive the upward movement of soil moisture. On the other hand, a zero flux condition is enforced at the top boundary. The soil hydraulic parameters of the test are given in Table 3.1. The upward migration of soil moisture is simulated for 3hrs and the results of pressure head distributions of HYDRUS and the proposed model are summarized in Figure 3.16 for various instances in time.
Figure 3.15. Comparison of pressure heads in TEST-1
Figure 3.16. Comparison of pressure heads in TEST-2
The results from Figure 3.16 clearly represent the high accuracy achieved by the proposed model in simulating the exfiltration behavior in an extremely dry soil that is saturated from below. This test is a perfect example to observe the movement of soil moisture towards the surface by overcoming the pull of gravity. It is even possible to see fully saturated conditions developing in the domain towards the end of the simulation (i.e., t>7200sec). Just like in Test-1, the position of the advancing front is accurately predicted by the proposed model in both space and time.

In the third test, the drainage in a 6m-long caisson is simulated for 100hrs to analyze the effect to gravitational drainage in soil-water distribution. To simulate this condition, an entirely saturated soil column (i.e., 0m pressure head initially) is let to drain due to gravitational pull. While a zero flux boundary condition is implemented at the top of the domain, the bottom of the domain is allowed to be saturated at all times and solved by a zero constant pressure head condition. The soil hydraulic parameters used in this test are given in Table 3.1. It is clearly seen from the table that the conductivity of the soil in this test is very high and represent a sandy soil which allows relatively faster movement of soil moisture. The pressure head distribution is simulated with both HYDRUS and the proposed model and the results are shown in Figure 3.17 for various instances in time.

The drainage of soil moisture in a long caisson is simulated for relatively extended periods of time compared to the other test cases. The vertical drainage of upper layers creates dry conditions and negative pressure heads. It is seen from Figure 3.17 that the proposed model simulates the temporal and spatial distribution of soil moisture accurately and gives almost identical results to HYDRUS model.

Finally, the proposed model is also tested against one of the simulations presented in the benchmark paper of Celia et al. (1990). The simulations are based on the van Genuchten model with a saturated hydraulic conductivity of 33.2cm/hr, saturated water content of 0.368, residual water content of 0.102 and $n$ and $\alpha$ values of 2.0 and 0.0335, respectively. Uniform initial conditions were set at -10m. The upper and lower boundaries are simulated with a -0.75m and -10m constant pressure head, respectively.

In this example, the intention of Celia et al. (1990) was to compare finite difference and finite element methods as well as the effect of temporal discretization. They have compared several simulations using different time steps with the results of a dense grid simulation. Therefore, the results of the proposed model are also compared to their dense grid simulation shown in Figure 3.18. It is clearly seen that the proposed model produces results that are very close to the dense grid results of Celia et al. (1990). Both the timing and position of the wetting front is properly positioned.
Figure 3.17. Comparison of pressure heads in TEST-3
The river bed is one of the most significant interfaces between surface and subsurface flow systems. The seepage along the river bed not only provides the minimum flow in the river during low flow periods but also attenuates the severity of flood event via bank storage during high flow episodes. It also supplies significant recharge to the aquifer when groundwater heads fall below the river bed. Due to its significance in regulating the river flows and in providing the much needed recharge to the aquifer, it is imperative to accurately analyze the characteristics of the two systems in a coupled fashion and quantify volumetric transfer between these two domains. In order to satisfy these objectives, a coupled surface-subsurface flow model is developed to link the one-dimensional channel flow with the two-dimensional vertically-averaged saturated groundwater flow. The following discussion closely follows the previous work of Gunduz and Aral (2003a, 2003b).

3.5.1. Coupling at River Bed

The lateral seepage flow between the channel flow and the groundwater flow domains provides the coupling mechanism at the river bed interface (Figure 3.19). The lateral flow term appears as a source/sink term in both the channel flow and the saturated groundwater
flow equations. The analysis of the lateral flow expression given in equation (3.7) reveals that lateral seepage flow is a direct function of river water surface elevation and groundwater head. Therefore, several possibilities occur depending on the relative values of the river water surface elevation and the groundwater head:

- \( h_r > h_g \)

  Seepage occurs from the channel to the groundwater flow domain. Hence, it becomes a lateral outflow for the channel flow model and an inflow for the groundwater flow model.

- \( h_r = h_g \)

  No seepage occurs between the two domains. Hence, the lateral inflow/outflow term in equations (3.1) and (3.29) becomes zero representing a no flux condition for both models.

- \( h_r < h_g \)

  Seepage occurs from the groundwater flow domain to the channel. Hence, it becomes a lateral inflow for the channel flow model and an outflow for the groundwater flow model.

![Figure 3.19. Channel flow / groundwater flow interaction](image)

Figure 3.19. Channel flow / groundwater flow interaction
One can see from these conditions that seepage is generally a head-dependent phenomenon for the coupled system. However, when the groundwater head falls below the bottom elevation of river sediments, second condition applies in equation (3.7) as the $(z_r - m_r)$ term becomes constant. It then becomes no longer a head-dependent phenomenon and seepage flow is treated as a constant flux condition within the numerical solution. It is, however, important to note that if the groundwater head falls too far below the channel, the link between the two systems is essentially broken and possibly an unsaturated transition zone would develop. Under such conditions, the analysis is no longer based on the first order gradient expression given in equation (3.7) and the entire coupling mechanism described herein must be modified.

It is also important to note that the coupling mechanism proposed in this study is based on the assumption that the movement of water at the river bed is at a steady state. If it can not be assumed that an equilibrium condition is reached at the river bed, this analysis would yield erroneous results. Under such circumstances, flow within the channel bed must be analyzed with a one-dimensional unsteady vertical flow model. However, the equilibrium assumption is valid for most large scale practical analysis of surface-subsurface flow interactions.

3.5.2. Proposed Simultaneous Solution Method

As discussed in Chapter 2, iterative (implicit) and non-iterative (explicit) coupling techniques are commonly used to establish the interactions between the surface and subsurface flow systems. While iterative algorithms are considered to be the most advanced coupling mechanisms for today’s modeler, they can be computationally costly for large systems due to the extra iteration loop in the solution. Moreover, they may be inaccurate at times when the convergence criterion is set at a high value to reduce computational run times.

Considering the limitations of current coupling mechanisms, a new simultaneous coupling technique is proposed by the author in an effort to link surface-subsurface flow systems at the river bed interface. The idea of the method is based on the simultaneous solution of the discretized forms of the two systems rather than the sequential solution that both the iterative and non-iterative coupling methods implement (Gunduz and Aral, 2003a). Although a theoretically similar approach might have already been applied in other branches of science, it is believed that the method is truly original in terms of its formulation in a coupled river-aquifer model framework.

The initial step for the simultaneous solution of the coupled model is discretizing the analysis domain. In this procedure, the channel network is discretized first considering the stability requirements of the channel flow model. Then, the groundwater flow domain is discretized considering the heterogeneity of the aquifer. During the discretization of the groundwater flow domain, each node of the channel flow model is selected such that it coincides with a node in the groundwater flow model as seen in Figure 3.20. This one-to-one correspondence of the nodes along the channel network is essential for the proposed
simultaneous solution of the coupled model (Gunduz and Aral, 2003a). If there is a requirement for finer discretization of the groundwater flow domain at any point along the channel network due to highly variable aquifer properties, the discretization of the channel flow model must also be modified to satisfy the one-to-one correspondence of the nodes. In this regard, the simultaneous solution of the coupled model is always based on finest discretized domain that either model enforces along the channel network (Gunduz and Aral, 2003a). For any other point in the analysis domain, the discretization is solely based on the requirements of the groundwater flow model.

The only exception to the one-to-one correspondence of nodes is observed at the channel junction points. At any junction with \( k \) inflowing channels and one outflowing channel, the numerical discretization of the channel flow model require that \( k+1 \) nodes are used to properly represent the \( k \) downstream boundary nodes of the inflowing channels and one upstream boundary node of the outflowing channel. Since all \( k+1 \) nodes physically represent the same junction point, they all correspond to a single point in the groundwater flow model. Therefore, at junction points, \( k+1 \) nodes of the channel flow model corresponds to one node of the groundwater flow model.

---

**Figure 3.20. Discretization of the domain**
The second step of the simultaneous solution of the coupled model is to write discretized equations of channel and groundwater flow equations. These are given in equations (3.26) and (3.46), respectively. When these equations are written for all nodes of channel and groundwater flow domains, a system of equations is obtained for both channel and groundwater flow system. At this point, if the standard iterative coupling scheme is implemented to solve this system, one would have two separate matrix solutions to solve each domain separately by using the latest values of the common parameter from the other domain (i.e., river water surface elevation for groundwater flow model and groundwater head for channel flow model). Following each solution, a convergence check is performed with respect to a pre-determined criterion. Once the check is satisfied the solution proceeds to the next time level. In the proposed simultaneous solution of the coupled model, however, the systems of equations obtained from the channel flow and groundwater flow models are assembled together within a single system so that they can be solved together in a simultaneous manner inside a single matrix structure. The assembled final matrix equation is shown in Figure 3.21. In the assembled global matrix equation, $A$ is the global coefficient matrix, $B$ is the global load vector and $x$ is the global unknown vector. As seen from Figure 21, the global matrix and vectors are obtained by combining their separate blocks obtained from channel and groundwater flow model. These separate blocks are written as:

\[
\begin{align*}
A^{GW} &= \alpha S^{j+1,k} + (1/\Delta t)M \\
A^{RIVER} &= J^{j+1,k} \\
B^{GW} &= \alpha F^{j+1,k} + (1-\alpha)F^j - (1-\alpha)S^j - (1/\Delta t)M \cdot \hat{h}_g^j \\
B^{RIVER} &= -f^{j+1,k} \\
x^{GW} &= \hat{h}_g^{j+1,k+1} \\
x^{RIVER} &= \delta x^{j+1,k+1}
\end{align*}
\]

![Figure 3.21. Global matrix equation and component blocks](image)

\[
\begin{bmatrix}
A^{GW} & 0 \\
0 & A^{RIVER}
\end{bmatrix}
\begin{bmatrix}
x^{GW} \\
x^{RIVER}
\end{bmatrix}
=
\begin{bmatrix}
B^{GW} \\
B^{RIVER}
\end{bmatrix}
\]
Although the global matrix is shown in full-matrix format, the calculations are performed using a banded matrix structure to reduce computer memory required to store and solve the system. The total bandwidth of the global matrix depends on the relative magnitudes of the bandwidths of channel flow and groundwater flow models. Therefore, the size of the global matrix is determined by the size of the bigger bandwidth. In general, the bandwidth of the groundwater flow model is bigger than the bandwidth of the channel flow model (Gunduz and Aral, 2003a).

It is crucial to emphasize that the global matrix solution directly solves the unknown variable in groundwater flow domain (i.e., hydraulic head) whereas it solves for the change in unknown variables between two iterations in channel flow domain (i.e., change in discharge and stage). Therefore, one has to evaluate the actual values of the unknown values after each solution of the global matrix equation before the global coefficient matrix and the load vector are re-assembled for the next solution. It is also important to note that since the global system is non-linear due to the non-linearities in channel flow and groundwater flow, it is solved several times for each time step until sufficient convergence is achieved for the unknown parameters. Hence, the global matrix solution involves an iterative portion to handle the non-linearity of the governing equations of both models. However, this iterative non-linear solution does not affect the simultaneous solution behavior of the overall coupled system. The iterative solution is only used to treat the non-linearity in the two sub-systems. The convergence of the non-linear solution is checked using two separate criteria for channel flow and groundwater flow components. Therefore, although the systems are solved together, the convergence of the solution is tested with respect to different criteria since the degree of the non-linearity in channel flow is generally much higher than the degree of non-linearity in groundwater flow. Typically, 2 to 3 iterations are found to be sufficient for the convergence of two sub-domain models (Gunduz and Aral, 2003a).

Even though the two hydrologic systems coupled in this model have significantly different time scales, their simultaneously coupled solution, unlike an iteratively coupled solution, requires a common time step in numerical discretization. Since the behavior of a channel flow model is generally more dynamic than the overall response of a groundwater flow model, this constraint could occasionally create long simulation periods with the proposed algorithm. However, it is always faster than the iterative solution approach that utilizes the same time step size (Gunduz and Aral, 2003a).

3.5.3. Model Testing

As there are no analytical solutions to verify against, two sets of hypothetical simulations are performed using the proposed model and the solution algorithm. In the first application, a hypothetical test case is simulated to test the model’s capabilities and limitations with a rectangular groundwater flow domain and an overlying single channel domain. In the second application, the same hypothetical test case is modified to analyze the model’s response with the presence of a channel network.
Single Channel-Aquifer System:

The coupled channel/groundwater flow model is first applied to a hypothetical single channel stream-aquifer system to demonstrate the performance of the proposed simultaneous solution algorithm. The physical setup of the hypothetical domain is shown in Figure 3.22. In this application, the stream is a 30m wide 10km long uniform rectangular channel with a constant slope of 0.0001m/m and divides the aquifer into two equal portions of 2000m wide on each side of the channel. The Manning’s roughness coefficient of the stream is uniform throughout the channel and has a value of 0.025. At steady flow conditions, the channel carries 100m$^3$/s discharge at the uniform flow depth of 3.56m. The thickness of the sediments at the bottom of the channel is 0.3m and the hydraulic conductivity of the deposits is 1.0E-6m/s. The channel bottom elevation at the most upstream point is given as 30m above mean sea level. To visualize results easily, the 10km long and 4 km wide unconfined aquifer is assumed to have a uniform and isotropic hydraulic conductivity of 1.0E-3m/s and the aquifer base is set at mean sea level. The stream flow model is discretized by 100m long elements giving a total of 101 nodes. The groundwater flow model domain is discretized by square elements with a side length of 100m giving a total of 4141 nodes and 4000 square elements. Furthermore, a constant time step of 1hr is used in simulations.

In the channel flow model, the upstream boundary condition for the channel is given by a trapezoidal discharge hydrograph with a base discharge of 100m$^3$/s, a peak discharge of 350m$^3$/s and a time to peak of 10 days (Figure 3.23). The downstream boundary condition is given by a single-valued rating curve that maps the discharge to its normal depth. In the groundwater flow model, the boundaries parallel to the stream are specified as constant head condition and the boundaries perpendicular to the stream are specified as no-flux condition. Moreover, the internal boundary, where the stream runs through, is specified as a head-dependent line source. The initial conditions in the stream flow model is given as uniform flow conditions (i.e., 100m$^3$/s of discharge and a corresponding 3.56m of depth) at all nodes. In the groundwater flow model, two different sets of initial hydraulic head surfaces are used. In the first simulation, the initial groundwater head in the aquifer is chosen to be at 32m at all nodes. This simulation illustrates a condition where lateral flow occurs from the stream to the aquifer. In the second simulation, the opposite scenario is simulated and the initial groundwater head in the aquifer is chosen to be 35m, illustrating a condition where the lateral flow occurs from the aquifer to the stream. These two simulations are referred to as Scenario-1 and Scenario-2, respectively and are abbreviated as S1 and S2 in the following discussion.
Figure 3.22. Physical setup of hypothetical domain, single channel
In both scenarios, the point comparisons of groundwater head and stream stage are presented in figures 3.23 and 3.25 at the mid point of the analysis domain (i.e., 5000m from the upper boundary of the aquifer, which also corresponds to the mid point of the stream). A spatial distribution of groundwater heads are also presented in figures 3.24 and 3.26 along the line (-2000m ≤ x ≤ 2000m; y = 5000m). Analysis of groundwater head time series in figures 3.23 and 3.25 reveals that the passage of the flood wave creates an increase in the groundwater heads by creating a mound near the river as long as the stream stages are higher than the groundwater heads for a sufficiently long period of time. This mound is the result of lateral inflow to the aquifer (Figure 3.24). It is also seen that the mound subsides and the bank storage is drained back to the stream when the stream stage falls below the groundwater heads. It is also seen from figures 3.23 and 3.25 that there is a lag between the peak values of the hydraulic head and the stream stage which clearly represents the dynamic behavior of the stream flow as opposed to the groundwater flow.

The response of the coupled system to a flood wave is directly related to the initial conditions in the stream and the aquifer. A comparison of figures 3.24 and 3.26 demonstrate the effect of initial groundwater head in the aquifer and its position relative to the stage in the stream. When the hydraulic head in the aquifer is higher than the stream stage (Figure 3.26), a discharge from bank storage occurs in the first 5 days of the simulation creating a drawdown near the stream. During the second 5 day period, stream stages increases due to the arrival of the flood peak and this creates a flow reversal towards the aquifer (Figure 3.26).

**Channel Network-Aquifer System:**

In the second application, the coupled channel/groundwater flow model is applied to a hypothetical stream network-aquifer system to demonstrate the performance of the proposed simultaneous solution algorithm to multiple channel applications. The physical setup of the hypothetical domain is shown in Figure 3.27. In this application, two stream channels (i.e., channels 1 and 2) meet and form a larger channel (i.e., channel 3) at the junction point shown in Figure 3.27. The two upstream tributaries are 30m wide and 7071m long uniform rectangular channels with a constant slope of 0.00015m/m. The downstream stream is 45m wide and 5000m long uniform rectangular channel with a constant slope of 0.0001m/m. The two upstream channels confluence at the mid-point of the domain and creates the junction. The Manning’s roughness coefficients of all channels are uniform throughout the domain and have a value of 0.025. At steady flow conditions, the two upstream channels carry 100m³/s whereas the downstream channel carries 200m³/s. The thickness of the sediments at the bottom of the channel is 0.3m and the hydraulic conductivity of the deposits is 1.0E-6m/s. To visualize results easily, the 10km long and 4 km wide unconfined aquifer is assumed to have a uniform and isotropic hydraulic conductivity of 1.0E-3m/s and the aquifer base is set at mean sea level. The stream flow model is discretized by variable length elements giving a total of 155 nodes. The groundwater flow model domain is discretized by quadrilateral elements with variable side lengths giving a total of 4161 nodes and 4022 elements. A constant time step of 1hr is used in simulations.
Figure 3.23. Groundwater head and river stage at the mid-point and river discharge at the upstream boundary for Scenario-1
Figure 3.24. Groundwater head profiles at various times along mid point for Scenario-1
Figure 3.25. Groundwater head and river stage at the mid-point and river discharge at the upstream boundary for Scenario-2
Figure 3.26. Groundwater head profiles at various times along mid point for Scenario-2
In the channel flow model, the upstream boundary conditions are given by a trapezoidal discharge hydrograph with a base discharge of 100 m$^3$/s, a peak discharge of 350 m$^3$/s and a time to peak of 10 days (Figure 3.29). The downstream boundary condition is given by a single-valued rating curve that maps the discharge to its normal depth. In the groundwater flow model, the boundaries parallel to the stream are specified as constant head condition and the boundaries perpendicular to the stream are specified as no-flux condition. Moreover, the internal boundary, where the stream runs through, is specified as a head-dependent line source. The initial conditions in the stream flow model are given as uniform flow conditions at all nodes. In the groundwater flow model, two different sets of initial hydraulic head surfaces are used. In the first simulation, the initial groundwater head in the aquifer is chosen to be at 32 m at all nodes. This simulation illustrates a condition where lateral inflow occurs from the stream to the aquifer. In the second simulation, the opposite scenario is simulated and the initial groundwater head in the aquifer is chosen to be 35 m, illustrating a condition where the lateral inflow occurs from the aquifer to the stream. These two simulations are referred to as Scenario-1 and Scenario-2, respectively and are abbreviated as S1 and S2 in the following discussion.

In both scenarios, the point comparisons of groundwater head and stream stage are presented in figures 3.28 and 3.32 at three points in the analysis domain. These points are shown in Figure 3.27. Among these three points, points 1 and 2 are on the left upstream channel and are situated 1745 m and 4537 m from the most upstream point of channel 1. On the other hand, point 3 is on the downstream channel and is situated at the mid point between the junction and the channel’s most downstream point (i.e., 2500 m from the junction). These three points are also positioned on the three transects depicted in Figure 3.27 (i.e., 1600 m, 4200 m, and 7500 m from the upper boundary of the aquifer). These transects are used to present the spatial distributions of groundwater heads along the aquifer.

Analysis of groundwater head time series in figures 3.29 through 3.31 and 3.33 through 3.35 reveal that the passage of the flood wave creates an increase in the groundwater heads by creating a mound near the river as long as the stream stages are higher than the groundwater heads for a sufficiently long period of time. This mound is the result of lateral inflow to the aquifer. It is also seen that the mound subsides and the bank storage is drained back to the stream when the stream stage falls below the groundwater heads. The spatial distribution of groundwater heads in transects 1 and 2 illustrate a symmetric response behavior since the physical characteristics of the upstream channels and their boundary conditions are exactly identical as a function of time. Any difference between these characteristics would clearly create an asymmetric hydraulic head distribution in the upper half of the aquifer.
Figure 3.27. Physical setup of hypothetical domain
In S1, the initial groundwater head in all three transects are below the initial river stages. This situation creates a lateral outflow from stream channels towards the groundwater domain, creating an increase in groundwater heads as seen in figures 3.29, 3.30 and 3.31. Then, the flood wave arrives and this increase is even more pronounced. Once the flood wave starts receding, the groundwater heads start falling. Since the water surface elevation decrease in channel is much more dynamic than the groundwater head decrease, a flow reversal is observed creating a lateral inflow to stream channels from the groundwater domain. This behavior is present in all transects after 15 days in figures 3.29, 3.30 and 3.31.

In S2, on the other hand, the initial groundwater head in all three transects are above the initial river stages. Hence, an immediate lateral inflow to the stream channels starts to develop. In the absence of a flood wave, this situation creates a decrease in groundwater heads in the immediate vicinity of the channels. Therefore, it is possible to observe the drawdown associated with this behavior in all transects in the first 5 days of the simulation in figures 3.33, 3.34 and 3.35. After the 5th day, the arrival of the flood wave forces an increase in the groundwater heads due to lateral outflow from the channel.

It is important to mention the fact that a relatively high hydraulic conductivity value and a relatively smoothly-increasing upstream discharge hydrograph are used to promote a rapid response behavior so that the results could be analyzed in a simpler and idealized fashion. In real time simulations, however, the aquifer conductivity values are generally much smaller and the hydrographs are commonly much steeper on the rising limb. Such a situation is presented in the application chapter of this study.


In addition to the river bed interface, surface and subsurface flows are also linked at the ground surface that has the largest areal extent for surface-subsurface interactions. Ground surface serves as the first point-of-contact for the incoming meteorological input and is the place where it is distributed into various components. It essentially provides the medium for runoff generation which makes it an important part of the hydrologic cycle. Furthermore, if a saturated-unsaturated zone separation is made in groundwater flow, like it has been done in this study, the water table would become another interface of importance to the hydrologist where unsaturated zone is divided from the saturated zone. In order to analyze the interactions between the overland flow zone, unsaturated groundwater flow zone and the saturated groundwater flow zone, a second coupled model is developed and presented in the following sections. This discussion closely follows the previous work of Gunduz and Aral (2003c).
Figure 3.28. Groundwater head and river stage at various points in domain and river discharge at the upstream boundary in Run-1
Figure 3.29. Groundwater head profiles at various times at transect-1 in Run-1
Figure 3.30. Groundwater head profiles at various times at transect-2 in Run-1
Figure 3.31. Groundwater head profiles at various times at transect-3 in Run-1
Figure 3.32. Groundwater head and river stage at various points in domain and river discharge at the upstream boundary in Run-2.
Figure 3.33. Groundwater head profiles at various times at transect-1 in Run-2
Figure 3.34. Groundwater head profiles at various times at transect-2 in Run-2
Figure 3.35. Groundwater head profiles at various times at transect-3 in Run-2
3.6.1. Coupling at Ground Surface and Water Table

In this second couple model, the infiltration/exfiltration flux between the overland flow and general groundwater flow domains provides the coupling mechanism at the ground surface and at the water table. A schematic of this model is shown in Figure 3.36. As seen from the figure, the overland flow domain is stacked on top an unsaturated zone which also lies above a saturated groundwater flow zone. This triple structure is dynamically linked to each other at the ground surface and at water table (Gunduz and Aral, 2003c).

Figure 3.36. Coupling at ground surface and water table
As groundwater flow domain is separated into a saturated and unsaturated zone, one should pay special attention to the interactions between these two systems. Depending on the moisture levels in the ground, the unsaturated zone may totally diminish if the water table rises to the surface. In this regard, while the overland flow and saturated groundwater flow domains exist continuously in this model, the presence and/or the extent of the unsaturated zone flow domain is a fully dynamic process and becomes a function of the corresponding hydrologic conditions over the land surface and below the water table. In essence, these dynamic conditions determine the existence of the ‘saturation from below’ or “saturation from above” mechanisms of overland flow generation and represent the highly dynamic behavior of surface-subsurface flow interactions.

In the setup shown in Figure 3.36, the overland flow and saturated groundwater flow discretizations coincide in the two-dimensional horizontal domain such that an overland flow node and a saturated groundwater flow node are located at the same x-y position. The soil column between these two nodes is considered to be the one-dimensional unsaturated zone. Therefore, the overall discretization yields a total of \( N \) unsaturated columns, where \( N \) is the total number of overland or saturated groundwater nodes. In this formation, it is important to note that the unsaturated zone columns are disconnected from each other and there is no flux in \( x \) or \( y \) directions. This approach is the foundation for the proposed quasi three-dimensional structure (Gunduz and Aral, 2003c). The alternative is a completely three-dimensional variably-saturated groundwater flow model coupled with the two-dimensional overland flow. In such a setup, the water table becomes a part of the solution and there is no deliberate separation between unsaturated and saturated groundwater flow zones. The fully three-dimensional groundwater flow model is, however, not suitable for large scale watershed modeling applications due to computational limitations associated with the three-dimensional nodal arrangement.

At the ground surface, overland flow model is coupled with the unsaturated zone model via the infiltration/exfiltration flux. Depending on the relative magnitudes of potential infiltration and water supply rate (i.e., the sum of rainfall rate and overland flow depth expressed as a rate within a time step), the top boundary condition of the unsaturated zone is set as a specified head or specified flux. Therefore, the unsaturated zone top boundary condition of the coupled model possibly switches from a specified head condition to a specified flux condition or vice versa within the course of a simulation (Gunduz and Aral, 2003c). When a specified flux condition is used at the top boundary of the unsaturated zone, the same flux value is also directly used in the overland flow equation. On the other hand, if a specified head condition is required at the top boundary, then the corresponding flux is evaluated according to Darcy’s law. The computed flux value is then used in the overland flow equation.

In a similar manner, the unsaturated and saturated zone groundwater flow models are linked to each other with the infiltration/exfiltration flux evaluated at the water table. In the setup shown in Figure 3.36, the bottom of the unsaturated zone is always fixed to be the water table. Hence, the boundary condition becomes a zero pressure head condition. The flux computed at the bottom of the unsaturated zone is then used as the infiltration/exfiltration
term in the saturated groundwater flow equation (Gunduz and Aral, 2003c). When the groundwater table elevation increases or decreases, the corresponding unsaturated zone depth decreases or increases, respectively. Consequently, the unsaturated zone discretization must be adjusted to the growing/shrinking domain size. This adjustment would require adding new nodes or removing existing nodes at the bottom of the domain when the water table moves down and up, respectively. In this regard, a sophisticated dynamic mesh update routine is integrated to the coupled model and the unsaturated zone mesh is updated at each time step of the simulation.

Although the initial idea was to implement the new simultaneous coupling idea in the solution of the current model, computational limitations became so severe that an iterative coupling idea had to be used. The unsaturated column between each overland/groundwater node couple increased not only the memory requirements of the model but also created extremely large matrices that were deemed impossible to solve within reasonable time frames. Consequently, the iterative coupling is used as an alternative solution method.

While one of the advantages of iterative coupling is the ability to use different time step sizes for each component of the model, the minimum time step requirement of all processes is used in solving all three components of the coupled model. Despite the increased run-times, this method is believed to better represent the influence of the highly dynamic behavior of the overland flow process on unsaturated zone flow process much. For all time steps, first the unsaturated zone model is solved for each column using the corresponding overland flow stage and groundwater head values from previous time step. As the spatial discretization in the unsaturated zone is updated at every time step according to the relative time-dependent positions of the water table, the domain is essentially constant within each time step. After obtaining the top and bottom fluxes from the unsaturated model, they are used as inputs to the overland and saturated groundwater models. Then, the overland and saturated groundwater flows are solved to find the overland flow depths and aquifer heads. Once the depths and water table elevations are computed, they are re-substituted to the unsaturated zone boundary condition values to solve all unsaturated zone columns again. This procedure is continued iteratively until sufficient convergence is achieved between two consecutive values of overland flow depth and groundwater head. Typically, one to two iteration cycles are sufficient to reach a converged solution due to the relatively slow response times of the saturated groundwater flow (Gunduz and Aral, 2003c).

3.6.2. Model Testing

The coupled model is applied to a rectangular test plot to demonstrate the performance of the different model components and the interactions in between. In this application, a 40 m wide and 500 m long rectangular plane (Figure 3.37) with a slope of 0.001 m/m in the longitudinal direction and 0.0 m/m in the transverse direction is used to model the response of a precipitation event shown in Figure 3.38. The response of the watershed is simulated for both sand and clay soils to demonstrate the effect of soil type on overland flow generation and groundwater recharge. The van Genuchten model parameters for both soils
are taken from the statistically averaged values given by Carsel and Parrish (1988) and given in Table 3.2.

Figure 3.37. Test bed modeling domain in coupled model-2

Figure 3.38. Precipitation event used in model
Table 3.2. Soil Hydraulic Parameters of Sand and Clay Soils (Carsel and Parrish, 1988)

<table>
<thead>
<tr>
<th></th>
<th>$\theta_s$ (-)</th>
<th>$\theta_r$ (-)</th>
<th>$\alpha$ (cm$^{-1}$)</th>
<th>n (-)</th>
<th>$K_s$ (cm/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SAND</td>
<td>0.430</td>
<td>0.045</td>
<td>0.145</td>
<td>2.680</td>
<td>29.70</td>
</tr>
<tr>
<td>CLAY</td>
<td>0.380</td>
<td>0.068</td>
<td>0.008</td>
<td>1.090</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Both the overland and saturated groundwater domains are discretized by square quadrilateral elements of 10m side length creating a total of 200 elements and 255 nodes (Figure 3.37). Each of these 255 unsaturated soil columns is discretized with a vertical spacing of 1 cm but the number of nodes varied during the solution according to the relative surface and groundwater table elevations for each column.

In the overland flow model, critical depth conditions are used at the outflow side of the domain and no flux conditions are used at all other sides of the domain. An initial flow depth of 1.0E-4m is used to remove numerical singularity at the first time step. In the saturated groundwater flow model, a fixed head condition is used beneath the outflow side of the overland flow model and no flux conditions are used at all other sides. A horizontal initial water table of 89.5 m is used in the simulation. The bottom boundary condition of the unsaturated zone is always taken to be a zero specified head condition at the water table. The top boundary condition, however, switches between a specified head and a specified flux condition depending on the presence of overland flow. An initial pressure head profile of -50 cm up to the capillary fringe of 3-4 cm is used to represent a moderately dry soil in all unsaturated soil columns. A constant time step of 1 sec is used in the simulation.

The following results are presented at three nodes (i.e., 13, 123, 243) in the two dimensional domain. These nodes represent an upstream, a midstream and a downstream point along the flow direction. The overland flow depth time series and the groundwater head time series of both soils are shown in figures 3.39 and 3.40, respectively. The unsaturated zone profiles at $t=9000$sec and $t=18000$sec of simulation are shown for nodes 13, 123 and 243 in figures 3.41, 3.42 and 3.43, respectively.

The simulations reveal that the selected rainfall event is intensive enough to create overland flow on both soil types. In the early stages of the simulation, the generated overland flow is governed by the saturation of the top soil layers and is therefore regarded as a “saturation from above” type overland flow. It is seen that the overland flow depths are larger in clay soils, which permits relative smaller amounts of infiltration compared to sandy soils. As seen from Figure 3.40, clay soil did not create any significant recharge to the groundwater since the hydraulic conductivity of clay is two orders of magnitude smaller than that of sandy soil. Consequently, considerable amounts of infiltration did not occur during the simulation period. On the other hand, it is seen from Figure 3.40 that sandy soil created significant recharge to the groundwater, particularly towards the downstream nodes where groundwater table reached very close to the surface. Hence, any further precipitation event
will likely create a “saturation from below” type overland flow especially in down slope, lowland area. Particularly, the unsaturated zone profile of node 243 shown in Figure 3.43 demonstrates the fact that such lowland areas get saturated in a faster rate than the upland areas and create a potential recharge zone for the groundwater domain. This finding is consistent with the generally accepted overland flow generation mechanisms where highland areas are mostly contribute to runoff via saturation from above and lowland areas are generally responsible for creating runoff via saturation from below (Dingman, 1994).

3.7. Analysis of Coupled Models

The sub-processes defining the hydrologic system are linked via the interfaces located at: (i) the groundwater table; (ii) ground surface; and, (iii) river bed. Of these, the river bed is the only interface which may have a certain thickness and may involve a sediment layer along the river bottom that may allow a delayed exchange between river and groundwater flow domains. All others are “zero-width” interfaces where water exchange occurs instantaneously. Although the river bottom sediment is considered to be a layered interface, it is assumed that the interactions occur instantly due to the relatively small thickness of the sediment layer. This assumption simplifies the overall coupling analysis (Aral and Gunduz, 2003).

An important aspect of integrating various sub-processes is the selection of the method applied to solve the matrix equations defining the system. Even though coupling via iterative solution and coupling via simultaneous solution are the most advanced levels of solving the sub-processes in an integrated fashion, iterative solution requires much smaller matrices to solve than the simultaneous solution. In iterative solutions, each sub-process model is integrated sequentially and solved separately by using the contributions from the other sub-processes. After each sub-model is solved, the common parameters linking these systems are checked for convergence (i.e., deviation from the previous iteration’s solution). If the solutions of these common parameters are not sufficiently close, the procedure is repeated until the differences between subsequent solutions are below a pre-determined convergence criteria. This iterative coupling idea is slow, especially when more than two sub-processes are linked together. On the other hand this approach would be less restrictive from the perspective of scaling concerns since each sub-process can possibly be analyzed within its own scale.

In simultaneous solution approach proposed in this study, all sub-process models are solved together using a common time step. In this approach all sub-model solution matrices are grouped in a single matrix structure and solved at once. Hence, this method requires the use of the smallest time step of all sub-models, which makes it impractical for the coupling processes requiring time steps from the two extremes (i.e., linking processes such as saturated groundwater flow and unsaturated groundwater flow). Attempting to solve such a system simultaneously results in very small time step requirements and creates numerical incompatibility between systems. On the other hand, this approach is more accurate than the iterative method since it does not involve improvement of the solution by iterating on the common parameters of the sub-models.
Figure 3.39. Overland flow depth time series in (a) sand and (b) clay soils at different nodes in the domain
Figure 3.40. Groundwater head time series in (a) sand and (b) clay soils at different nodes in the domain
Figure 3.41. Unsaturated zone profiles of clay and sand soils at an upstream node (Node 13) at $t=9000$sec and $t=18000$sec
Figure 3.42. Unsaturated zone profiles of clay and sand soils at a midstream node (Node 123) at $t=9000\text{sec}$ and $t=18000\text{sec}$
Figure 3.43. Unsaturated zone profiles of clay and sand soils at a downstream node (Node 243) at t=9000sec and t=18000sec
The wide array of time scales required to efficiently simulate the flow pathways is the most important problem of the watershed modeling. The incompatibility of the sub-process time scales makes the overall coupling of the system difficult and sometimes impractical. As described before, unsaturated flow numerically requires small time steps in the order of seconds to describe the vertical movement of moisture in the unsaturated domain where as the groundwater flow can be run with time steps in the order of days. If a simultaneous solution technique is used to couple these two systems, then the entire system would need to be run with the time step of the unsaturated zone. This condition is computationally costly and inefficient for the groundwater flow simulation. Moreover, including the entire unsaturated zone discretization to the overall matrix structure would simply make the matrix sizes impractical to solve with current computational power, which is why the second coupled model discussed above is not solved with the simultaneous solution approach.

Nevertheless, regardless of the method used, it is the understanding of the author that coupling of a process requiring large time steps with a process requiring small time steps over a large watershed application is still not practical with the current level of computational power. Small time step requirements of certain processes including the unsaturated zone and overland flow zone practically create very large simulation times to simulate watershed scale events (i.e., large areal extent and long temporal periods). When this is the case, certain engineering judgments are to be made to either simplify or totally neglect the processes that create the bottle neck. Although these judgments might violate the proper representation of the system, it would still allow the modeler to gain an insight of the system with optimal model performance. It is believed, without these shortcuts, large scale watershed modeling is still not feasible when distributed models are used in sub-process modeling and non iterative solution processes are selected in solving the integrated model.

The problem of spatial scale compatibility between models is not as significant as the problem of time scale compatibility which is discussed above. The spatial scale compatibility becomes most significant within the simultaneous solution framework where sub-processes must be discretized to have common nodes. In the first model discussed above (i.e., coupled river/groundwater flow model), the system is composed of a common set of nodes representing the river discretization, which are also a member of the unconfined aquifer discretization. The corresponding dependent variables of both models (i.e., river water surface elevation and the groundwater head) at these nodes essentially perform the simultaneous coupling. While the iterative coupling method does not require having common nodes, it would still be more convenient for the modeler to work with two dependent variables at the same point without the need to go through the task of interpolation.

The situation is much worse in the second coupled model discussed above (i.e., coupled overland flow/unsaturated zone/saturated zone model). Similar spatial scale compatibility issues become more pronounced within the solution of this model. Coinciding overland and
saturated groundwater nodal points are used to effectively link the vertical distance between the groundwater table and ground surface with an unsaturated zone model with variable nodal points. The coinciding nature of nodal points is required to have an unsaturated zone in between and to guarantee correct volume balance within the unsaturated zone model. However, it is impractical to use the many discretized unsaturated zone nodes between each node-couple of overland/saturated zone model and solve a huge system matrix at each time step, a simultaneous solution algorithm is definitely not the method of choice with current level of computer speed.

3.8. Hybrid Model

The analysis of the two coupled models reveals some key features that have to be addressed for accurate understanding of the system. The problems associated with the scales of subprocesses and their coupled counterparts are probably the most significant difficulty in integrated watershed modeling. As shown in sections 3.5 and 3.6, it is theoretically possible to couple all processes if computational cost is not an issue. However, for large scale applications such as catchment modeling, the small scale requirements of overland and unsaturated zone flow domains exhibit severe limitations on efforts in fully integrating the system (Aral and Gunduz, 2003). Furthermore, the issues discussed in Chapter 2 further complicate the large scale applications of both overland and unsaturated zone flow modeling. Consequently, a hybrid modeling approach is proposed in this study in which distributed and lumped parameter models are essentially linked and blended to obtain a semi-distributed watershed model. In such models, the overland flow and unsaturated zone models are replaced with their lumped parameter empirical counterparts in an effort to simplify the overall analysis. When issues like computational limitations, proper mathematical formulation of physical processes and data requirements are addressed accurately and sufficiently, these systems would be included in the analysis as shown in sections 3.5 and 3.6.
4. Coupled Contaminant Transport Model

In this chapter, a coupled contaminant transport model that is based on the proposed hybrid flow model given in Chapter 3 is presented. The coupled contaminant transport model is one of the earliest attempts of multi-pathway contaminant transport phenomena. It essentially links the surface and subsurface transport processes and couples them in a semi-simultaneous manner. The difficulties associated with the numerical solution of the advection dispersion equation would presently not allow fully simultaneous coupling of these transport processes.

4.1. One Dimensional Channel Transport Model

4.1.1. Governing Equations

The mathematical model of the one-dimensional channel contaminant transport is given by the mass conservation equation including extra terms for lateral mass contribution from overland and seepage flows. As the contribution from seepage flows is not considered in previous studies, this study can be considered as a first attempt to incorporate the impact of subsurface transport on surface transport of contaminants. In addition, the following governing equation not only considers the effect of advective seepage transport but also formulates a dispersive component of transport as a first order Fickian process over the thickness of the river bed. With these additions, the one-dimensional advection dispersion equation in channel flow can be written by using a control volume approach and presented in the following conservation form:

\[
\frac{\partial(C_r A)}{\partial t} + \frac{\partial}{\partial x} \left( V A C_r \right) - \frac{\partial}{\partial x} \left( A D_L \frac{\partial C_r}{\partial x} \right) + k C_r A - q_{L1} C_{L1}^* + n_{sed} D_{sed} \frac{C_r - C_r}{m_r} w_r - q_{L2} C_{L2}^* = 0 \tag{4.1}
\]

where \( x \) is the longitudinal coordinate representing the distance along the channel, \( t \) is the temporal coordinate, \( C_r \) is the contaminant concentration in the channel, \( A \) is flow area, \( V \) is the cross-section averaged flow velocity, \( D_L \) is the longitudinal dispersion coefficient in the channel, \( k \) is the decay coefficient, \( q_{L1} \) and \( q_{L2} \) are the lateral seepage and overland flows per channel length (positive for inflow and negative for outflow), \( C_{L1}^* \) and \( C_{L2}^* \) are the contaminant concentration associated with lateral seepage and overland flows, respectively, \( n_{sed} \) is the porosity of the sediment layer, \( D_{sed} \) is the vertical dispersion coefficient in the sediment layer, \( m_r \) is the thickness of the sediment layer and \( w_r \) is the wetter perimeter of the river. It is important to note that the values of \( C_{L1}^* \) and \( C_{L2}^* \) change according to the direction of the lateral flow terms such that when lateral flow is towards the channel (i.e., inflow to the channel), these values take the associated concentrations coming from the groundwater (i.e., \( C_g \)) and overland flow domains (i.e., \( C_o \)) whereas as they become the concentration in the channel (i.e., \( C_r \)) when the lateral flow is away from the channel (i.e., outflow from the channel):
The value of the longitudinal dispersion coefficient is an important parameter in the overall distribution of the contaminant within the channel network. It may become the major transport mechanism in mildly moving or stagnant sections of the channel such as ponds or small tributary inflow sites to the main channel. Although the exact way to obtain the value of the longitudinal dispersion coefficient is to perform tracer tests, it is only available for selected reaches of only a small number of rivers. Therefore, water quality modelers often use empirical formulations that are mainly based on the easily measured hydraulic and channel characteristics. Following the early works of Taylor (1954) and Elder (1959), numerous researchers including Fischer (1966, 1968, 1975, 1979), McQuivey and Keefer (1974), Liu (1977) and Aral et al. (1980) have developed methods to estimate the longitudinal dispersion coefficient. Their research were later followed by Magazine et al. (1988), Iwasa and Aya (1991), Kousis and Rodriguez-Mirasol (1998), Seo and Cheong (1998), Deng et al. (2001) and Kashefipour and Falconer (2002), who have also developed both semi-analytical and empirical equations for estimating the longitudinal dispersion in river channels. Despite the vast amount of published work, there is no globally accepted formulation that is used extensively. In this study, the most recent study conducted by Kashefipour and Falconer (2002) is implemented. They have analyzed the available data via regression analysis and proposed their version of an empirical formula for the longitudinal dispersion coefficient that can be written as:

\[
C_{L1}^* = \begin{cases} 
C_r & \text{when } q_{L1} < 0 \\
C_g & \text{when } q_{L1} > 0 
\end{cases} 
\]  

(4.2)

\[
C_{L2}^* = \begin{cases} 
C_r & \text{when } q_{L2} < 0 \\
C_o & \text{when } q_{L2} > 0 
\end{cases} 
\]  

(4.3)

\[
D_L = 10.612 \left( \frac{V}{V^*} \right) Vd 
\]  

(4.4)

where \(d\) is the water depth in the channel and \(V^*\) is the shear velocity defined as:

\[
V^* = \sqrt{gR_s S_f} 
\]  

(4.5)

They have obtained a coefficient of determination value of 0.84 for a data set including more than 30 major rivers in the United States. Following comparisons with the results obtained from Seo and Cheong’s equation (Seo and Cheong, 1998), they have decided to combine the two equations in a linear manner to estimate the longitudinal dispersion coefficient more accurately. By trial and error and comparison of predicted vs. measured dispersion coefficients, they proposed the following form of the equation as their second formulation for dispersion coefficient:
\[ D_L = \left[ 7.428 + 1.775 \left( \frac{B}{d} \right)^{0.620} \left( \frac{V}{V^*} \right)^{0.572} \right] \left( \frac{V}{V^*} \right) V d \]  

(4.6)

Upon further investigations with the two alternative forms, Kashefipour and Falconer (2002) recommended the use of the first equation for open channel flows with B/d ratios in excess of 50 and the use of second equation for open channel flows with B/d ratios less than 50.

4.1.2. Initial Conditions

In order to start the transient solution, initial values of the contaminant concentration are to be specified along the one-dimensional channel domain such that:

\[ C_r(x,0) = C_{ro}(x) \]  

(4.7)

where \( C_{ro} \) is the initial concentration distribution along the channel network.

4.1.3. Boundary Conditions

Similar to the one-dimensional channel flow model, the contaminant transport model also have two different types of boundary conditions specified at (i) external; and, (ii) internal boundaries of the domain. The external boundary conditions are given at the most upstream and downstream points of the channel network whereas the internal boundary conditions are specified at internal junction points of the channel network.

4.1.3.1. External Boundary Conditions

In this study, the contaminant transport model can accommodate several upstream boundary conditions and a single downstream boundary condition. Thus, the model does not solve looped channel networks. At any upstream boundary, a specified concentration time series can be used as the boundary condition. The concentration time series is either available from continuous measurement (i.e., specified concentration) or from simple contaminant mass loading computation (i.e., specified mass flux):

\[ C_r(0,t) = C_{ru}(t) = \frac{M(t)}{Q(t)} \]  

(4.8)

where \( M(t) \) is the mass loading rate from some upstream source, \( Q(t) \) is the river flow at the upstream boundary and \( C_{ru} \) is the corresponding upstream boundary concentration time series. At the downstream boundary, a zero concentration gradient is generally used as the boundary condition when the boundary is far away from the contaminant zone:
\[ AD \frac{\partial C}{\partial x} \bigg|_{x=I_d} = 0 \]  

which states that advection dominates at the outflow and the contaminant propagates out of the domain unhindered. When the boundary is not far and the outflow concentration is measured, a specified total mass flux, \( f \), is used as the downstream boundary condition:

\[ QC - AD \frac{\partial C}{\partial x} \bigg|_{x=I_d} = f \]  

4.1.3.2. Internal Boundary Conditions

Any two or more channels intersecting within a channel network forms a junction where internal boundary conditions are specified to satisfy the contaminant mass balance. In this study, the proposed contaminant transport model follows its flow counterpart and does not allow for looped networks. Hence, it requires that there is always a single outflow channel from a junction. The mass balance equation at a junction can then be specified as:

\[ \sum_{k=1}^{m} A_k J_k - A_o J_o = \frac{dM}{dt} \]  

where \( m \) is the total number of inflowing channels to the junction, \( J_k \) and \( A_k \) are the total mass flux and the area at the end of the \( k^{th} \) inflowing channel to the junction, \( J_o \) and \( A_o \) represent the total mass flux and the area at the beginning of the outflowing channel from the junction, and \( dM/dt \) corresponds to the change in mass within the junction. Following the basic assumption applied in many modeling applications, the change in mass storage within a junction is assumed to be negligible compared to the change in mass within in a channel. Consequently, the mass balance equation can be written as:

\[ \sum_{k=1}^{m} A_k J_k - A_o J_o = 0 \]  

Furthermore, the continuity of concentration at the junction guarantees that all the concentrations must be equal to each other at the junction:

\[ (C_r)_k = (C_r)_o \quad k = 1,2,\ldots,m \]  

4.1.4. Numerical Solution Scheme

There are numerous numerical solution techniques for solving advection dispersion equation. These techniques can be classified as: (i) Eularian methods including finite difference, finite element or finite volume methods; (ii) Lagrangian methods; and, (iii)
Hybrid methods. When the limitations of these methods discussed in Chapter 2 are considered, it is still tempting to use fixed grid methods for the solution of the advection dispersion equation. One of the key criteria behind this selection lies in the fact that the flow model that would supply the necessary flow data to the contaminant transport model is based on a Eulerian framework. Therefore, information obtained from the flow model at fixed points can best be used in the transport model at the same grid points. Hence, the one-to-one correlation of flow and transport model discretizations greatly simplifies the implementation of the contaminant transport model and possibly increases its accuracy since it would not require unnecessary interpolations that would otherwise be inevitable. Furthermore, systematic modeling of complex channel networks is still only viable with fixed-grid methods.

Based on this discussion, the advection-dispersion equation describing the transport of contaminants in a river channel is solved using a fixed grid control-volume finite difference scheme. In the context of this scheme and similar other fixed grid methods, it is widely accepted by the numerical modeler that the dispersion component of the equation could generally be solved without any problems using a variety of schemes. The problem generally arises from the advection component of the equation, particularly for highly advective transport of contaminants with sharp fronts, where the numerical methods start to lose accuracy and computational efficiency. While dispersion favors implicit solution algorithms with possible use of large time steps, advection modeling generally utilizes an explicit algorithm with time steps limited by the Courant number criteria. Hence, the two major contaminant transport processes essentially behave in a contradicting manner. Since dispersion modeling could also be done with an explicit algorithm, a fully explicit scheme for the entire ADE is possible. However, such a scheme would not allow a simultaneous solution for the transport equation in river with the transport equation in groundwater and is not favorable for this study. Rather, the matrix solution of implicit schemes is necessary to simultaneously solve the two transport systems. The only exception to this setup would be the problematic advection component of the river transport that should be solved using an explicit scheme. It is this motivation that forces to separate the two processes and solve them in two steps. Using a fairly recent development in the area that results in the formulation of the so-called ‘split operator’ approach, one can now separate the advection operator from the dispersion and the rest of the operators and solve them using the most suitable scheme possible for each operator. Although this approach appears to be a violation of the principle of “simultaneous presence” of these processes in nature, it provides a very powerful technique to handle the numerical difficulties associated with each particular operator. Essentially, this procedure provides a sound methodology that gives mathematically identical results to the traditional compact operator methods. Consequently, one could discretize the equation by evaluating the advection term explicitly in time and the remaining terms implicitly in time. The discretized form of the equation would then become:
\[(C_i^+)^{j+1} = (C_i)^j + \Delta t \left[ -\frac{\partial}{\partial x} (VAC_i) \right] \]
\[+ \Delta t \left[ \frac{\partial}{\partial x} \left( AD_L \frac{\partial C_i}{\partial x} \right) - kC_i A \right. \]
\[+ q_{L1}C_{L1}^* - n_{sed} D_{sed} \frac{C_g - C_i}{\Delta z} w_e + q_{L2}C_{L2}^* \left\] \]

which gives cell-average values of \((C_i, A)\) in each control volume, \(i\), at the future time line \(j+1\), based on the cell-average values of \((C_i, A)\) in each control volume at the current time line \(j\), as well as the mass influx and outflux to/from the control volume. The square brackets represent some form of spatial discretization. Since the advection term is treated explicitly, the equation may be rewritten in two substeps without compromising the algorithmic integrity:

\[(C_i^+)^* = (C_i)^j + \Delta t \left[ -\frac{\partial}{\partial x} (VAC_i) \right] \]
\[(C_i^+)^{j+1} = (C_i)^* + \Delta t \left[ \frac{\partial}{\partial x} \left( AD_L \frac{\partial C_i}{\partial x} \right) - kC_i A \right. \]
\[+ q_{L1}C_{L1}^* \]
\[\left. - n_{sed} D_{sed} \frac{C_g - C_i}{\Delta z} w_e + q_{L2}C_{L2}^* \right] \]

In essence, this procedure of splitting the operators first allows the fluid to advect for a time step then lets it to disperse and decay in its new advected location. With this approach, it is possible to use a suitable solution scheme for advection and other operators. In this regard, the highly accurate Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms (QUICKEST) algorithm could be used to model the advection operator, while the dispersion operator is discretized with a standard central difference scheme. The remaining terms are just algebraic terms evaluated at the \((j+1)\)th time line. The details associated with the discretizations of the advection operator with the QUICKEST scheme and the dispersion operator with the central difference scheme are given in Gunduz (2004). The formulations of the boundary conditions as well as the treatment of the junctions are also given in this appendix. Using the formulations given in Gunduz (2004), the channel transport equation becomes:
\[ (C_r A)_i^{j+1} = (C_r A)_i^* \]

\[ + \frac{\Delta t}{0.5 (\Delta x_{i-1} + \Delta x_i)} \left[ \left( A_L^{j+1} (D_L)_j \right)_i \left( \frac{(C_r)_i^{j+1} - (C_r)_i^{j+1}}{\Delta x_i} \right) \right] - \left( A_L^{j+1} (D_L)_j \right)_i \left( \frac{(C_r)_i^{j+1} - (C_r)_i^{j+1}}{\Delta x_{i-1}} \right) \]

\[ + \Delta t \left[ -k (C_r)_i^{j+1} A_L^{j+1} + (q_{L1})_i^{j+1} \left( C_{L1}^* \right)_i^{j+1} \right. \]

\[ - \left( n_{sed} D_{sed} \right)_i \left( \frac{(C_g)_i^{j+1} - (C_r)_i^{j+1}}{\Delta z} \right) \left( w_r \right)_i^{j+1} + (q_{L2})_i^{j+1} \left( C_{L2}^* \right)_i^{j+1} \] (4.17)

where \((C_r A)^*\) is the result of advection operator using the explicit QUICKEST algorithm as given in Gunduz (2004).

4.1.5. Model Testing

The one-dimensional channel contaminant transport model is tested against the available analytical solutions in a single channel framework. Since there are no analytical solutions that define the transport of contaminants in a channel network, model testing of contaminant transport in channel networks is performed by a number of supplementary tests for various hypothetical conditions of pure advection and pure dispersion.

The single channel verification of the proposed channel contaminant transport model is done with the exact solution originally developed by Ogata and Banks (1961) and later modified by Bear (1972) and van Genuchten and Alves (1982). The original one-dimensional mathematical model is written as:

\[ \frac{\partial C_r}{\partial t} + V \frac{\partial C_r}{\partial x} - D_L \frac{\partial^2 C_r}{\partial x^2} + kC_r = 0 \] (4.18)

that defines not only the advective-dispersive transport but also the first order decay of contaminants in a simple channel. The initial and boundary conditions of the problem can also be given as:

\[ C_r(x,0) = C_o \quad \text{for} \quad x \geq 0 \]

\[ C_r(0,t) = \begin{cases} C_{ru} & \text{for} \quad 0 < t < t^* \\ 0 & \text{for} \quad t \geq t^* \end{cases} \] (4.19)

\[ \frac{\partial C_r}{\partial x}(x,t) = 0 \quad \text{for} \quad t \geq 0 \]

which defines the conditions for a continuous source of a finite duration, \(t^*\). The analytical solution of this problem for conservative species \((k=0)\) can then be written as:
\[ C_r(x,t) = \begin{cases} 
C_o + (C_{ru} - C_o) A(x,t) & 0 < t \leq t^* \\
C_o + (C_{ru} - C_o) A(x,t) - C_{ru} A(x,t-t^*) & t > t^* 
\end{cases} \]  
(4.20)

where:

\[ A(x,t) = \frac{1}{2} \text{erfc} \left( \frac{x-Vt}{\sqrt{4D_L t}} \right) + \frac{1}{2} \exp \left( \frac{Vx}{D_L} \right) \text{erfc} \left( \frac{x+Vt}{\sqrt{4D_L t}} \right) \]  
(4.21)

For non-conservative species \((k \neq 0)\), the solution is slightly modified as:

\[ C_r(x,t) = \begin{cases} 
C_o A(x,t) + C_{ru} B(x,t) & 0 < t \leq t^* \\
C_o A(x,t) + C_{ru} B(x,t) - C_{ru} B(x,t-t^*) & t > t^* 
\end{cases} \]  
(4.22)

where the functions \(A(x,t)\) and \(B(x,t)\) are defined as:

\[ A(x,t) = \exp(-kt) \left[ 1 - \frac{1}{2} \text{erfc} \left( \frac{x-Vt}{\sqrt{4D_L t}} \right) - \frac{1}{2} \exp \left( \frac{Vx}{D_L} \right) \text{erfc} \left( \frac{x+Vt}{\sqrt{4D_L t}} \right) \right] \]  
(4.23)

\[ B(x,t) = \frac{1}{2} \exp \left( \frac{Vx}{2D_L} (1-\Gamma) \right) \text{erfc} \left( \frac{x-Vt\Gamma}{\sqrt{4D_L t}} \right) + \frac{1}{2} \exp \left( \frac{Vx}{2D_L} (1+\Gamma) \right) \text{erfc} \left( \frac{x+Vt\Gamma}{\sqrt{4D_L t}} \right) \]  
(4.24)

The term \(\Gamma\) in function \(B(x,t)\) is given as:

\[ \Gamma = \sqrt{1 + \frac{4kD_L}{V^2}} \]  
(4.25)

To test the proposed model with the analytical solution given above, a hypothetical rectangular channel setup is created so that steady uniform flow will prevail in the channel at all times. A constant discharge of 10\(\text{m}^3/\text{s}\) is passed through a 10000\(\text{m}\) long rectangular channel that has a base width of 20\(\text{m}\). The channel lies on a 0.001\(\text{m/m}\) bed slope and carries the discharge at a uniform depth of 0.5\(\text{m}\) with a constant velocity of 1\(\text{m/s}\). Initially, the channel is assumed to contain no contaminants. A constant specified concentration boundary condition of 1\(\text{mg/L}\) is implemented at the upstream boundary of the channel. The contaminant is allowed to advect, disperse and/or decay within the channel as a function of time. The results of numerical simulations and analytical solutions are compared in figures 4.1 through 4.6.
Figure 4.1. Comparison of numerically simulated and analytically computed concentrations in an advection dominated flow ($D_L=1.0E^{-8} \text{ m}^2/\text{s}$)
Figure 4.2. Comparison of numerically simulated and analytically computed concentrations in a moderate dispersion flow ($D_L=30 \text{ m}^2/\text{s}$)
Figure 4.3. Comparison of numerically simulated and analytically computed concentrations in a high dispersion flow ($D_L=100 \text{ m}^2/\text{s}$)
Figure 4.4. Comparison of numerically simulated and analytically computed concentrations in an advection dominated flow ($D=1.0\times10^{-8} \text{ m}^2/\text{s}$) with decay ($k=3.0\times10^{-4} \text{ s}^{-1}$)
Figure 4.5. Comparison of numerically simulated and analytically computed concentrations in a moderate dispersion (D=10 m²/s) flow with moderate decay (k=1.0E⁻⁴ s⁻¹)
Figure 4.6. Comparison of numerically simulated and analytically computed concentrations in a moderate dispersion ($D_L=10 \text{ m}^2/\text{s}$) flow with high decay ($k=3.0\times10^{-4} \text{ s}^{-1}$).
In the first set of tests, the basic transport characteristics of the contaminant are analyzed and the decay of the contaminant is not allowed. Three different tests are performed with different dispersion coefficients representing (i) an essentially pure advection flow with very low dispersion ($D_L=1.0E-8$ m$^2$/s); (ii) a medium dispersion ($D_L=30$ m$^2$/s) flow; and, (iii) a high dispersion ($D_L=100$ m$^2$/s) flow. The numerically simulated vs. analytically computed results are compared in figures 4.1, 4.2 and 4.3. In the first test shown in Figure 4.1, a very small amount of dispersion is allowed and the contaminant transport is mainly an advection dominated event. It can be seen that the pattern and timing of the sharp front is properly captured with the proposed model in three different positions in time. Hence, it is possible to conclude that the model can accurately simulate advection dominated contaminant transport. The second test is performed with moderate amount of dispersion which represents most of the flow patterns found in nature. As seen in all three time positions presented in Figure 4.2, the simulated results are either identical or very close to the analytical solution. Therefore, it can be concluded that the proposed model accurately captures the expected advection and dispersion patterns of the contaminant plume. Finally in the third test, simulations are performed with a significantly high dispersion value. The dispersion coefficient is so high that the plume shows a ±3000m deviation from its center of gravity (Figure 4.3). Similar to the previous two tests, the comparison of simulated and calculated results also reveals an excellent fit and demonstrates the prediction power of the proposed model.

In the second set of tests, the basic transport characteristics of the contaminant are analyzed under the influence of contaminant decay. Three different tests are performed with different dispersion and decay coefficients representing (i) a high decay rate in an essentially pure advection flow ($k=3.0E-4$ s$^{-1}$); (ii) a low decay rate in a medium dispersion flow ($k=1.0E-4$ s$^{-1}$); and, (iii) a high decay rate in a medium dispersion flow ($k=3.0E-4$ s$^{-1}$). The numerically simulated vs. analytically computed results are compared in figures 4.4, 4.5 and 4.6. As seen from the figures, the simulated and calculated results are almost identical or very close to each other which represent the predictive capabilities of the proposed model with decay. In all three cases, decay acts as an additional smoothing mechanism on the sharp contaminant profile that is already evened out with the dispersion.

In a channel network setup, there are no analytical solutions that the model could be tested against when advection, dispersion and/or decay are the governing mechanisms of fate and transport. It is, however, possible to perform simple benchmark tests when the steady uniform channel flow only allows advection of contaminants. Although such a situation is of no practical value, it is believed to provide an important test condition for the numerical model within a network setup. To test the simulation capabilities of the proposed model in a channel network under simple advection, a three channel network with two upstream tributaries and a downstream channel is used as shown in Figure 4.7.
Figure 4.7. Simple channel network for testing pure advective transport

The hypothetical channel network consists of three 10000m long rectangular channels laid on a 0.001m/m bed slope. The upstream tributaries and the downstream main channels have top widths of 20m and 40m and carry a discharge of 10m$^3$/s and 20m$^3$/s, respectively. The steady uniform flow creates a normal depth of 0.5m and a velocity of 1m/s in all three channels. Initially, all channels contain zero contaminant concentration. Then, the first tributary starts to receive constant 1mg/L while the second tributary gets constant 3mg/L throughout the rest of the simulation period of 0.2 days. Since flow in the channel system is steady and uniform and advection is the only means of transport, it is expected that the two concentration streams blend in the junction and travel downstream with the volumetric average concentration. Considering the fact that both tributaries carry an equal amount of discharge, the blended main channel concentration is expected to balance out at 2mg/L and still continue to travel downstream as a step function based on the assumption that the mixing of two streams occur instantaneously. The results of numerical simulation exactly follow this intuitive expectation and shown in Figure 4.8 for two time positions representing before and after blending of two streams.
Although the channel network would not allow a similar intuitive analysis for pure diffusion/dispersion, the proposed model is still used to simulate the channel network shown in Figure 4.7 so that the results could at least be analyzed from a general perspective. In this test, however, the second tributary is taken to be free from contamination and is assumed to have a zero concentration boundary condition at the most upstream point. Since the second tributary does not carry any contaminant, one would expect dispersion towards not only along the main channel but also towards the second tributary once the contaminant reaches the junction. Therefore, a symmetric pattern is expected beyond the junction. The results of pure diffusion/dispersion test verify this expectation as shown in Figure 4.9. The contaminant is allowed to diffuse from the upstream point of the first tributary for 30 days and the corresponding contaminant concentration is calculated at all points along the channel network. It is important to note that this test is performed with a diffusion coefficient of 10m^2/s, which corresponds to an unrealistically high diffusion coefficient since dispersion is not a transport mechanism in stagnant water. It is, however, convenient to test the numerical functioning of the code rather than drawing any physical results. The results clearly demonstrate the symmetric behavior beyond the junction and follow an error function trend. It is therefore possible to conclude that the proposed model functions properly in the case of pure diffusion in a channel network setup.

4.2. Two Dimensional Saturated Groundwater Transport Model

4.2.1. Governing Equations

The governing equation for contaminant transport in a two-dimensional vertically-averaged groundwater flow is obtained by vertically integrating the general three-dimensional conservation of mass equation in the groundwater. The equation is later on modified to include the effect of line source/sink following the original idea proposed by Gunduz and Aral (2004a). For an anisotropic, non-homogeneous unconfined aquifer with principle permeability directions not matching the coordinate directions, the governing equation of contaminant transport in groundwater is given by:
Figure 4.8. Pure advective transport in a channel network
Figure 4.9. Pure diffusion/dispersion in a channel network
\[
\begin{align*}
&nR_d \left( h_g - z_b \right) \frac{\partial C_g}{\partial t} + \left( h_g - z_b \right) q_x \frac{\partial C_g}{\partial x} + \left( h_g - z_b \right) q_y \frac{\partial C_g}{\partial y} \\
&- \frac{\partial}{\partial x} \left[ \left( h_g - z_b \right) nD_{xx} \frac{\partial C_g}{\partial x} \right] - \frac{\partial}{\partial y} \left[ \left( h_g - z_b \right) nD_{yy} \frac{\partial C_g}{\partial y} \right] \\
&- \frac{\partial}{\partial y} \left[ \left( h_g - z_b \right) nD_{yx} \frac{\partial C_g}{\partial x} \right] - \frac{\partial}{\partial y} \left[ \left( h_g - z_b \right) nD_{xy} \frac{\partial C_g}{\partial y} \right] \\
&+ I \left( C^* - C_g \right) + \lambda nR_d \left( h_g - z_b \right) C_g + K_w n \left( h_g - z_b \right) C_g - C_g S_y \frac{\partial h_g}{\partial t} \\
&+ \sum_{k=1}^{n_w} \left[ Q_{w,k} \left( C^*_{w,k} - C_g \right) \delta \left( x - x_{w,k} \right) \delta \left( y - y_{w,k} \right) \right] \\
&+ \sum_{m=1}^{n_r} \left[ \int_0^1 q_{L1,m} \left( C^*_{L1,m} - C_g \right) - n_{sed,m} D_{sed,m} \frac{C_{r,m} - C_g}{m_r} \left( w_r \right)_m \right] \right] = 0
\end{align*}
\]  

(4.26)

where \( x \) and \( y \) are the spatial coordinates in the horizontal domain, \( t \) is the temporal coordinate, \( C_g \) is the vertically-averaged contaminant concentration, \( n \) is the porosity of the medium, \( q \) is the vertically-averaged Darcy flux, \( D \) is the hydrodynamic dispersion coefficient, \( h_g \) is the vertically-averaged hydraulic head, \( z_b \) is the elevation of the bottom imperious layer, \( I \) is the infiltration/exfiltration rate (i.e., positive for exfiltration and negative for infiltration), \( C^* \) is the contaminant concentration associated with the filtrating water, \( \lambda \) is the radioactive decay constant for a radioactive contaminant, \( K_w \) is the biochemical decay constant for a biodegradable contaminant, \( S_y \) is the specific yield of the unconfined aquifer, \( n_w \) is the number of wells in the domain, \( Q_{w,k} \) is the well flow rate of the \( k \)th well located at \((x_{w,k}, y_{w,k})\) in the domain (i.e., positive for a discharging well and negative for an injecting well), \( C^*_{w,k} \) is the contaminant concentration associated with the \( k \)th well, \( \delta \) is the Dirac Delta function, \( n_r \) is the number of river channels in the domain, \( q_{L1,m} \) is the lateral seepage flow rate of the \( m \)th river channel (positive for outflow from the aquifer or inflow to the river and negative for inflow from the aquifer or outflow from the river), \( C^*_{L1,m} \) is the contaminant concentration associated with the \( m \)th river channel, \( C_{r,m} \) is the contaminant concentration in the \( m \)th river channel, \( n_{sed} \) is the porosity of the sediment layer, \( D_{sed} \) is the vertical dispersion coefficient in the sediment layer, \( m_r \) is the thickness of the sediment layer, \( w_r \) is the wetted perimeter of the \( m \)th river channel, \( g_{x,m} \) and \( g_{y,m} \) are the Cartesian coordinate components of the parametric equation defining the \( m \)th river channel in the domain, \( u \) is the dimensionless parameter of the parametric equation and \( R_d \) is the retardation coefficient given by:

\[
R_d = 1 + \frac{\rho K_d}{n}
\]  

(4.27)
where $\rho_b$ is the bulk density of the porous medium and $K_d$ is the portioning coefficient. It is important to note that the values of $C^*_i$, $C^*_{w,k}$ and $C^*_{L,m}$ change according to the direction of the volumetric flux driving the mass transport. Accordingly, when the volumetric flux is towards the aquifer, these values take the associated concentrations in the infiltrating water (i.e., $C_I$), the well recharge (i.e., $C_{w,k}$) and the lateral seepage flow (i.e., $C_{r,m}$) where as they become the concentration in the groundwater (i.e., $C_g$) when the corresponding volumetric fluxes are away from the aquifer:

$$
C^*_i = \begin{cases} 
C_g & \text{when } I > 0 \\
C_I & \text{when } I < 0 
\end{cases} \quad \text{(exfiltration)} \quad (4.28)
$$

$$
C^*_{w,k} = \begin{cases} 
C_g & \text{when } Q_{w,k} > 0 \\
C_{w,k} & \text{when } Q_{w,k} < 0 
\end{cases} \quad \text{(discharging well)} \quad (4.29)
$$

$$
C^*_{L,m} = \begin{cases} 
C_g & \text{when } q_{L,m} > 0 \\
C_{r,m} & \text{when } q_{L,m} < 0 
\end{cases} \quad \text{(outflow from aquifer)} \quad (4.30)
$$

Despite the vast number of alternative empirical formulations in open channels, the theory of dispersion is much better developed in groundwater systems. The developed equations are generally globally accepted and implemented in many modeling applications. The theory is based on the concept of a hydrodynamic dispersion coefficient that is defined as the sum of mechanical dispersion and molecular diffusion. Bear (1972) has formulated the hydrodynamic dispersion coefficient as:

$$
D = \tau D_m + \alpha_L v 
$$

where $\tau$ is the tortuosity of the medium, $D_m$ is the molecular diffusion coefficient, $\alpha_L$ is the longitudinal dispersivity and $v$ is the average pore velocity defined by the ratio of Darcy velocity and porosity of the medium. When the relative importance of mechanical dispersion and molecular diffusion is studied, it is seen that the mechanical dispersion is almost always the major contributor of hydrodynamic dispersion coefficient under field conditions. In the last 30 years, Bear’s analysis has become the industry standard for the analysis of dispersion in groundwater systems, which describes the following three-dimensional dispersion tensor:

$$
D_{ij} = D_m \tau \delta_{ij} + \alpha_L |v| \delta_{ij} + (\alpha_L - \alpha_T) \frac{v_i v_j}{|v|} 
$$

where $\alpha_L$ and $\alpha_T$ are the longitudinal and transverse dispersivities, respectively, and $\delta_{ij}$ is the Kronecker delta. In a vertically-averaged two-dimensional setup, the hydrodynamic dispersion coefficient reduces to a second order tensor and is given as:
\[ D_{xx} = \alpha_L \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + D_m \tau \]

\[ D_{yy} = \alpha_T \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + D_m \tau \]

\[ D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{v_x v_y}{v} \] (4.33)

4.2.2. Initial Conditions

The initial values of the contaminant concentration, \( C_{g0} \), are specified as the initial conditions of the groundwater contaminant transport model:

\[ C_g(x, y, 0) = C_{g0}(x, y) \] (4.34)

which is generally taken to be zero representing a contaminant release into an otherwise uncontaminated domain or is obtained from: (i) field measurements, (ii) a steady state contaminant transport simulation; and, (iii) a previous unsteady model solution.

4.2.3. Boundary Conditions

Two different types of boundary conditions can be specified along different external boundaries of the groundwater domain. Type-1 or specified concentration boundary conditions are used to model boundaries with known contaminant concentration values. It is also known as a Dirichlet boundary condition and is given as:

\[ C_g(x, y, t) = C_{gd}(x, y, t) \] (4.35)

where \( C_{gd} \) is the known concentration. It is also possible to define a variable boundary condition, which becomes a zero dispersive flux for a volumetric outflow and a specified mass influx for a volumetric inflow:

\[ -n \cdot \left[ (h_g - z_b) n D \cdot \nabla C_g \right] = 0 \quad \text{for} \quad (h_g - z_b) q \cdot n > 0 \]

\[ (h_g - z_b) n \cdot \left[ q C_g - n D \cdot \nabla C_g \right] = (h_g - z_b) q_v C_v \quad \text{for} \quad (h_g - z_b) q \cdot n < 0 \] (4.36)

where \( q_v \) is the volumetric inflow rate and \( C_v \) is the contaminant concentration in the inflowing stream.
4.2.4. Numerical Solution Scheme

Although the form of the groundwater contaminant transport equation is very similar to the channel transport equation, the difficulties associated with the numerical solution are not as significant as the channel transport equation. This finding is mainly due to the fairly small advection velocities that govern the groundwater transport. The relative magnitudes of the advective and dispersive transport mechanisms are much closer to each other than their counterparts in channel flow. Hence, fixed grid finite element and finite difference models are still widely applied in groundwater transport modeling. Similar to its flow counterpart, the finite element method became a popular method due to the flexibility it offers in simulating aquifer domains with irregular boundaries as well as heterogeneous aquifer properties. In this regard, the Galerkin finite element method based on the method of weighted residuals is used in this study to solve the groundwater contaminant transport. The weak form of the problem is developed by Gunduz (2004). Using the same discretization that its flow counterpart uses; the contaminant transport model also implements linear interpolating functions and quadrilateral elements. The resulting finite element matrix equation obtained by applying the Galerkin procedure is given as:

\[
S \cdot \dot{\mathbf{C}}_g + M \cdot \frac{d \mathbf{C}_g}{dt} = \mathbf{F}
\]  (4.37)

where \( S \), \( M \) and \( F \) stand for global stiffness matrix, global mass matrix and global load vector, respectively, and \( \dot{\mathbf{C}}_g \) is the approximate contaminant concentration vector. These global matrices and vectors are obtained by tiling their element counterparts according to the connectivity of elements within the solution domain. The explicit formulas of element matrices and vectors are derived in Gunduz (2004). The element integrals are evaluated with the same numerical integration scheme used in the flow model.

The ordinary differential in (4.37) is obtained as a result of finite element discretization and can be solved using a number of techniques including the one-step finite difference approximations. Since the concentration is a function of time, it is possible to define two positions, \( j \) and \( j+1 \), representing the known and unknown time lines, respectively. If one defines an intermediate point between the known and the unknown time line (i.e., \( j+\alpha \) where \( 0 \leq \alpha \leq 1.0 \)), then the corresponding concentration could be calculated as a weighted average:

\[
\mathbf{C}_{g,j}^{j+\alpha} = \alpha \mathbf{C}_{g,j}^{j+1} + (1 - \alpha) \mathbf{C}_{g,j}^j
\]  (4.38)

such that if the intermediate point is selected as the mid point between the two time lines (i.e., \( \alpha=0.5 \)), the concentration becomes an arithmetic average of the two concentrations at two ends. Following the same procedure used in the flow model, one can obtain the final form as:
Since the transport equation is linear, solution does not require a non-linear solver as its flow counterpart does and the equation given above is solved by a suitable linear matrix solver.

4.2.5. Model Testing

Similar to its flow counterpart, there are no documented analytical solutions for the unsteady groundwater contaminant transport in two dimensions. Therefore, the proposed model is tested against the analytical solutions developed within a one dimensional framework. The analytical solution is very similar to the one showed in channel contaminant transport with the slight modification with respect to the retardation coefficient. Following the works of Ogata and Banks (1961) and van Genuchten and Alves (1982), the one-dimensional mathematical model for groundwater contaminant transport is written as:

\[ R \frac{\partial C_g}{\partial t} + \frac{q}{n} \frac{\partial C_g}{\partial x} - D \frac{\partial^2 C_g}{\partial x^2} + K_w C_g = 0 \]  

(4.40)

in which advection, dispersion and decay are three mechanisms of fate and transport. The initial and boundary conditions of the problem can also be given as:

\[ C_g(x, 0) = C_o \quad \text{for} \quad x \geq 0 \]

\[ C_g(0, t) = \begin{cases} C_{gD} \quad \text{for} \quad 0 < t < t^* \\ 0 \quad \text{for} \quad t \geq t^* \end{cases} \]  

(4.41)

\[ \frac{\partial C_g}{\partial x}(x, t) = 0 \quad \text{for} \quad t \geq 0 \]

which defines the conditions for a continuous source of finite duration. The analytical solution of this problem for conservative species \((K_w=0)\) is slightly modified from the solution of channel transport and is written as:

\[ C_g(x, t) = \begin{cases} C_o + (C_{gD} - C_o) A(x, t) \quad \text{for} \quad 0 < t \leq t^* \\ C_o + (C_{gD} - C_o) A(x, t) - C_{gD} A(x, t - t^*) \quad \text{for} \quad t > t^* \end{cases} \]  

(4.42)

where the function \(A(x,t)\) is now written as::

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For non-conservative species ($K_w \neq 0$), the solution is given as:

$$C_g(x,t) = \begin{cases} 
C_o A(x,t) + C_{gd} B(x,t) & 0 < t \leq t^* \\
C_o A(x,t) + C_{gd} B(x,t) - C_{gd} B(x,t-t^*) & t > t^*
\end{cases}$$  \hspace{1cm} (4.44)

where the functions $A(x,t)$ and $B(x,t)$ are defined as:

$$A(x,t) = \exp \left( -\frac{K_d t}{R_d} \right) \left[ 1 - \frac{1}{2} \text{erfc} \left( \frac{R_d x - (q_x / n)t}{\sqrt{4D_x R_d t}} \right) - \frac{1}{2} \exp \left( \frac{(q_x / n)x}{D_x} \right) \text{erfc} \left( \frac{R_d x + (q_x / n)t}{\sqrt{4D_x R_d t}} \right) \right]$$  \hspace{1cm} (4.45)

$$B(x,t) = \frac{1}{2} \exp \left( \frac{(q_x / n)x}{2D_x} (1 - \Gamma) \right) \text{erfc} \left( \frac{R_d x - (q_x / n)t \Gamma}{\sqrt{4D_x R_d t}} \right) + \frac{1}{2} \exp \left( \frac{(q_x / n)x}{2D_x} (1 + \Gamma) \right) \text{erfc} \left( \frac{R_d x + (q_x / n)t \Gamma}{\sqrt{4D_x R_d t}} \right)$$  \hspace{1cm} (4.46)

The term $\Gamma$ in function $B(x,t)$ is given as:

$$\Gamma = \sqrt{1 + \frac{4K_u D_x}{(q_x / n)^2}}$$  \hspace{1cm} (4.47)

To test the proposed model with the analytical solution given above, a two-dimensional hypothetical rectangular aquifer is created so that steady uniform flow will prevail in the aquifer at all times. The 100m long aquifer is structured in such a way that the flow is essentially one-dimensional in the two dimensional domain between two fixed head boundaries creating a hydraulic gradient of 0.1m/100m. The unconfined aquifer flow would then result in a constant Darcy velocity of 1.0E-5m/s when a uniform hydraulic conductivity value of 0.01m/s is used throughout the domain. The relative values of the aquifer conductivity and hydraulic gradient are deliberately selected to be on the high end to allow rapid response from the aquifer. In the following tests, a retardation coefficient of 1.2 and two dispersion coefficients of 1.0E-4m$^2$/s and 1.0E-5m$^2$/s are used in the simulations. Moreover, a decay coefficient of 1.0E-6s$^{-1}$ is also used to simulate the removal of contaminants from the aquifer. The simulations used a specified constant contaminant
concentration of 1mg/L as the boundary condition of the transport module. On the opposite side of the domain, a zero concentration gradient boundary condition is implemented. The contaminant is allowed to advect, disperse and/or decay within the channel as a function of time. The results of numerical simulations and analytical solutions are compared in figures 4.10 through 4.13.

The numerical solution demonstrates perfect fit with the analytical solution for both moderate and low dispersion flows. Since high dispersion flows are always easier to simulate than low dispersion flows, it is not difficult to predict that dispersion values higher than the ones used herein will not possess any problems. For pure advection flows, however, the spatial and temporal discretization used in these simulations must be further refined or more sophisticated higher order numerical algorithms must be implemented to avoid numerical oscillations. Such conditions are not common and as problematic as it is in channel flow due to significantly lower advection velocities observed in groundwater flow. The simulated and computed results also demonstrate very good fit when 1.0E-6s⁻¹ of decay is added to the simulation. Therefore, the proposed model performs accurately when simulating contaminant transport in saturated groundwater flow domain.

4.3. **Coupled Surface-Subsurface Contaminant Transport Model**

Even though there are many discrete contaminant transport models that describe the fate and transport of contaminant in rivers and aquifers, no coupled analysis has ever been attempted before to the best of the author’s knowledge. In this regard, this study is believed to be one of the earliest efforts to couple a surface and subsurface contaminant transport process.

The proposed coupled surface-subsurface transport model follows the hybrid approach discussed in Chapter 3. The two systems are coupled at the river bed using both the advective and the dispersive transport mechanisms. These mechanisms provide possible pathways for the transfer of contaminants between the two domains. This is one of the crucial points of the proposed contaminant transport model since one or both of these mechanisms might be working to transport the contaminant. In previous studies of contaminant transport modeling in discrete systems, only the advective transport mechanism is considered where the impact of other domains is included as source/sink terms possibly due to its relatively larger contribution compared to dispersive transport. Although this approach is reasonable when the interactions with other domains are only vaguely attempted and the focus is on one particular domain, it might yield to an incorrect treatment of the simultaneous interactions if the dispersive component is neglected from the analysis.
Figure 4.10. Comparison of numerically simulated and analytically computed concentrations for $D_x=1.0E-4 \text{ m}^2/\text{s}$
Figure 4.11. Comparison of numerically simulated and analytically computed concentrations for $D_x=1.0E-5$ m$^2$/s
Figure 4.12. Comparison of numerically simulated and analytically computed concentrations for $D_x = 1.0 \times 10^{-4} \text{ m}^2/\text{s}$ and $K_w = 1.0 \times 10^{-6} \text{ s}^{-1}$
Figure 4.13. Comparison of numerically simulated and analytically computed concentrations for $D_x=1.0E-5$ m$^2$/s and $K_w=1.0E-6$ s$^{-1}$.
4.3.1. Coupling at the River Bed

In this analysis, the total mass flux along the river bed interface is considered to be a function of (i) the groundwater hydraulic head; (ii) river water surface elevation or stage; (iii) contaminant concentration in the river; and, (iv) contaminant concentration in the groundwater:

\[ \text{Total mass flux} = f(h_r, h_g, C_r, C_g) \]  \hspace{1cm} (4.48)

While the first two of these parameters determine the magnitude and the direction of the advective flux, the remaining two is responsible for the magnitude and the direction of dispersive flux. The vectorial sum of advective and dispersive fluxes would then give the total mass flux between the two domains. It is important to note that the advective flux is a direct function of the water flow between the two domains and is always in the direction of the lower head. As the values of river water surface elevation and the groundwater head changes dynamically, the direction of the volumetric flux and the advective transport changes consequently. On the other hand, the dispersive flux is a function of the concentration gradient and is always towards the domain with lower contaminant concentration based on the Fickian description of dispersion. The direction of the dispersive flux also changes when the contaminant concentration in the channel or in the aquifer changes. This situation represents a highly variable transport phenomenon and is a strong function of the dynamically varying flow conditions. Based on this discussion, one of the following alternative conditions would describe the interactions between the river and the aquifer at all times:

- \[ h_r > h_g \text{ and } C_r > C_g \]
  Both the advective and the dispersive fluxes are towards the aquifer since the river stage is larger than the groundwater head and the concentration in river is larger than the concentration in groundwater.

- \[ h_r > h_g \text{ and } C_r < C_g \]
  The advective flux is towards the aquifer since the river stage is larger than the groundwater head. The dispersive flux, on the other hand, is towards the river since the groundwater domain has a higher contaminant concentration than river.

- \[ h_r < h_g \text{ and } C_r > C_g \]
  The advective flux is towards the river since the groundwater head is larger than the river stage. The dispersive flux, on the other hand, is towards the aquifer since the river has a higher contaminant concentration than the aquifer.
• \( h_r < h_g \) and \( C_r < C_g \)

Both the advective and the dispersive fluxes are towards the river since the groundwater head is larger than the river stage and the concentration in groundwater is larger than the concentration in river.

• \( h_r = h_g \) and \( C_r > C_g \)

The advective flux does not exist since both heads are equal. The dispersive flux is the only available transport mechanism and it is towards the aquifer since the concentration in river is larger than the concentration in aquifer.

• \( h_r = h_g \) and \( C_r < C_g \)

The advective flux does not exist since both heads are equal. The dispersive flux is the only available transport mechanism and it is towards the river since the concentration in aquifer is larger than the concentration in river.

• \( h_r > h_g \) and \( C_r = C_g \)

The dispersive flux does not exist since both domains have the same contaminant concentrations. The advective flux is the only available transport mechanism and it is towards the aquifer since the river stage is larger than the groundwater head.

• \( h_r < h_g \) and \( C_r = C_g \)

The dispersive flux does not exist since both domains have the same contaminant concentrations. The advective flux is the only available transport mechanism and it is towards the river since the groundwater head is larger than the river stage.

• \( h_r = h_g \) and \( C_r = C_g \)

Both the advective and the dispersive flux do not exist and there is no mass transfer between the two domains.

In any one of the cases discussed above, the total mass flux is the summation of the relative contributions from advective and dispersive components. In general, the advective transport mechanism is much larger than the dispersive transport mechanism. Therefore, the direction of the total mass flux typically follows that of the volumetric flux. Only under the condition that the river water surface elevation is in equilibrium with the groundwater head, the dispersive flux dominates the transport phenomenon.

It is important to note that the coupling mechanism for the contaminant transport model is similar to that proposed in the flow model. It is also based on the assumption that the
vertical movement of contaminants at the river bed is at a steady state. If it is not possible to assume that an equilibrium condition is reached at the river bed, this analysis would yield erroneous results. Under such circumstances, contaminant transport within the channel bed must be analyzed with a one-dimensional unsteady vertical transport model at the river bed. However, the equilibrium assumption is valid for most large scale practical analysis of surface-subsurface interactions.

The coupling of the contaminant transport model is provided with a modified form of the new simultaneous solution algorithm discussed in Chapter 3. Although the algorithm could have been directly used as discussed in flow coupling, the numerical solution of the advective transport mechanism enforced an explicit solution algorithm which in turn violated the full simultaneous coupling of the surface and subsurface flow processes. When an equally accurate implicit algorithm is devised to solve the advection mechanism of channel transport model, one can apply the fully simultaneous coupling of Chapter 3. Until that time, a semi-simultaneous algorithm is implemented in this study. In the proposed semi-simultaneous algorithm, the advection mechanism of channel contaminant transport model is solved as a separate event prior to the other processes. In a sense, water packet is first advected to its new position in channel. Then, the dispersion, source/sink and decay mechanisms of the channel transport model are solved in a fully simultaneous manner with all mechanisms of the groundwater transport model.

4.3.2. Model Testing

The proposed coupled contaminant transport model is applied to a hypothetical river/aquifer system to demonstrate its performance and the proposed semi-simultaneous solution algorithm. The numerical mesh of the problem is shown in Figure 4.14. In this figure, two densely meshed regions are identified for detailed analysis. In this application, the stream is a 20m wide 5km long uniform rectangular channel with a constant slope of 0.0001m/m and a Manning’s roughness coefficient of 0.020. At steady flow conditions, the channel carries 100m$^3$/s discharge at the uniform flow depth of 4.12m. The thickness of the sediments at the bottom of the channel is 0.3m and the hydraulic conductivity of the deposits is 7.0E-6m/s. The river lies at the center of a 5km long and 0.8km wide unconfined aquifer which is formed by clay and gravel layers. The clay layer is located at the center of the aquifer (600≤x≤1400 and 2400≤y≤4700) and has a hydraulic conductivity value of 5.5E-8m/s. Two gravel layers are located to the north (600≤x≤1400 and 1000≤y≤2400) and south (600≤x≤1400 and 4700≤y≤6000) of the clay layer and have a hydraulic conductivity value of 1.0E-3m/s.

The hydraulics of the aquifer is arranged so that it would be a discharging aquifer at the upstream portions of the river and a recharging aquifer at the downstream portions of the river as shown in Figure 4.15. With this particular setup, it is possible to analyze the potential of the river to serve as a fast transport medium for contaminants in the aquifer. Accordingly, any contaminant plume in the vicinity of the upstream reaches of the river will first be transported to the river and will then be quickly conveyed to the lower portions
of the aquifer where the reversed seepage flow direction will reintroduce the contaminants to the aquifer.

Figure 4.14. Physical setup of hypothetical domain
In this setup, the hydraulics of the river is of little concern and is driven by a steady 100m$^3$/s discharge at the upstream boundary throughout the simulation period. At the downstream boundary, a normal depth boundary condition is implemented. The hydraulics of the aquifer shown in Figure 4.15 is governed by fixed head boundary conditions on left and right boundaries and no flux conditions at the top and bottom boundaries. Hence, the aquifer feeds the river in the upper 2500m of the river whereas the river feeds the aquifer in the lower 2500m of the river. Therefore, any contaminant introduced from the upper region will first reach the river, transported with river flow and later reintroduced to the aquifer in the lower region.

Figure 4.15. Hydraulic head distribution and flux pattern within the domain
In this study, a contaminated area covering a 20m by 20m area is located at the upper densely meshed zone centered at (900,5400) as shown in Figure 4.14. This zone is called the upper analysis zone in the following discussion and covers a 100m X 100m area on the left bank of the river. It is assumed that the contaminated area located at the core of the zone continuously releases a conservative contaminant of 1.0E+5mg/L throughout the simulation. Due to the dominant aquifer flow towards the river, the contaminant plume is then transported towards the river mainly by advective transport. Along the river bed, the contaminant passes through the bed sediments and pollutes the otherwise pristine river water. From this point of contamination, the contaminant is transported further downstream by river flow and quickly affects the lower portions of the aquifer. The analysis is focused on the lower portions of the aquifer on the lower densely meshed area located 3.5km downstream from the original contamination area. This region covers a 300m X 300m area and is centered at position (1000,1950) as shown in Figure 4.14. It is also called the lower analysis zone in the following discussion. The migration of contaminant in upper and lower analysis zones are analyzed as a function of time.

Before reviewing the results, it is important to stress that fact that the physical setup shown in Figure 4.14 and discussed above is deliberately chosen to demonstrate the impact of a river passing through a contaminated aquifer. In general, it is well known that the travel time of a contaminant in an aquifer could easily be in the order of tens of years to cover a distance of a couple of kilometers under favorable geological settings. The purpose of this application, however, is to show that this commonly accepted belief might be totally wrong with the presence of a river in the system and suitable hydrological conditions.

Following the introduction of the contaminant, it is transported towards the river mainly due to the advective transport governed by the general flow field in the upstream portions of the aquifer where seepage velocities are observed to be in the order of 3.0E-5m/s due to high conductivity value of gravel and large hydraulic head gradient between the boundaries of the aquifer and the river. The contaminant then starts to seep into the river waters where it is heavily diluted and transported downstream. The analysis reveals that the contaminant concentration underneath the river reaches a value of 2.0E+4mg/L in less than 25 days. After the contaminant reaches the river, it only takes about 0.8hrs to reach the point of analysis in the downstream reaches of the river due to the 1.2m/s average flow velocity in the river. Therefore, the river acts as a conduit for rapid transport of contaminants. The hydraulic head conditions in the lower portions of the aquifer favors seepage inflow to the aquifer as shown in Figure 4.14. This hydrologic pattern re-introduces the contaminants to the otherwise uncontaminated portions of the aquifer. It must be mentioned that, without the river, the contamination in the aquifer can not reach the lower analysis zone which is located about 3.5km downstream. Furthermore, the clay layer in between the two gravel layers acts as an additional barrier for the contamination to reach the lower analysis zone even in long time periods.

First, the migration of the contaminant towards the river is analyzed as shown in Figure 4.16. The spatial distribution of time-dependent change in contaminant concentration in the upper analysis zone reveals the fact that contaminant quickly reaches the river due to the
large advective and dispersive transport. The advection velocity in this zone is in the order of $7.0\times 10^{-5}$ m/s, which allows the contaminant to move about 6 m/day. Moreover, the dispersivity of the medium is taken to be 50 m, which also significantly contributes to the overall rapid movement of the contaminant. As soon as the contaminant reaches the river, it starts to cross the river bed via advective and dispersive transport and mix into the river waters. At this point, the advective transport is a function of the lateral seepage velocity whereas the dispersive flux is based on the concentration gradient between the two domains. It is important to note that the dilution effect of the river is generally significant since it is a function of river discharge and total seepage from the aquifer. The contaminant concentration distribution in the river is shown in Figure 4.17 as a function of time and space. From this figure, it is seen that the river concentration is effectively constant from the point where the contamination zone is located as there is no reaction involved. The amount of dispersion in the channel allows it to migrate backwards towards the upstream boundary of the channel where a zero concentration is specified.

Due to the fast travel times in the river channel, the contaminant is quickly transported downstream where it finds an opportunity to seep back into the aquifer according to the hydraulic head distribution in the region. However, the large dilution in the river removed the strength of the contaminant and is at least 5 orders of magnitude smaller when reintroduced to the aquifer. The spatial distribution of time-dependent change in contaminant concentration in the lower analysis zone is shown in Figure 4.18. Since the river acts as a line source for the otherwise pristine lower zone of the aquifer, the contaminant migrates almost perpendicular to the governing flux direction.
Figure 4.16. Spatial distribution of time-dependent change in contaminant concentration in upper analysis zone
Figure 4.17. Time-dependent change in contaminant concentration in river
Figure 4.18. Spatial distribution of time-dependent change in contaminant concentration in lower analysis zone
5. Model Application to Lower Altamaha Watershed

In this chapter, the coupled flow and contaminant transport model developed earlier is applied to a large scale watershed to demonstrate the versatility and applicability of the proposed modeling system in a field application using site specific field data. The selected watershed is located in southern Georgia and is a part of the greater Altamaha river basin. The flow model is calibrated and verified with field data from several gaging stations operated by the U.S. Geological Survey. The transport model is then applied with this flow solution to test the consequences of various scenarios based on different contaminant loading conditions. These applications demonstrate the potential use of the model developed in this study in understanding and evaluating the environmental impacts of critical contaminant loading conditions in this watershed which is a relatively pristine watershed otherwise.

5.1. Data Requirements of the Proposed Model

The proposed model requires significant amounts of data mainly due to the distributed nature of the hydrologic and hydraulic processes modeled as well as the physics-based representation of the fundamental flow and contaminant transport laws defining these processes. For the successful application of the proposed model, these data requirements must be satisfied accurately and realistically. The model data is stored in several input files that are organized according to the flow pathway and characteristics. All files are standard text files with special formatting applied for easy preparation and retrieval of the data. A list of the required data files for flow and transport model are given in Table 5.1.

The common data files (i.e., general_data.txt and time_data.txt) are used by both flow and transport models. The time parameters file specify the temporal simulation data including the starting and ending date and time as well as maximum, minimum and standard time steps to be used in variable time stepping algorithm. The minimum and maximum iteration boundaries used to alter the time step are also specified in the time parameters file. The general data file specifies the use of the model (i.e., flow simulation or flow and transport simulation) and the convergence criteria for transport model.

The flow parameters in the channel and groundwater flow domains are specified in RIVflow_parameters.txt and GWflow_parameters.txt, respectively. These files include the total number of flow related parameters such as the total number of nodes, elements, boundary conditions, lines sources and wells in the groundwater flow domain as well as the total number of cross-sections, channels, junctions, data lines, overland flow contributions and boundary conditions in the channel flow domain. These files also include the tolerance values for the associated non-linear solvers.
Table 5.1. Data files for the Proposed Model

<table>
<thead>
<tr>
<th>Component</th>
<th>Module</th>
<th>Data file</th>
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<tr>
<td>Main</td>
<td>Common module</td>
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<td></td>
<td></td>
<td>general_data.txt</td>
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<tr>
<td>Flow Model</td>
<td>Channel flow module</td>
<td>RIVflow_parameters.txt</td>
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<td>RIVflow_junction_data.txt</td>
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<td>RIVflow_initial_cond.txt</td>
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<td>Overland_flow.txt</td>
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<td>Boundary condition data files*</td>
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<td></td>
<td>Groundwater flow module</td>
<td>GWflow_parameter.txt</td>
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<td>GWflow_nodes.txt</td>
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<td>GWflow_lines.txt</td>
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<td>GWflow_wells.txt</td>
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<td>Boundary condition data files*</td>
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* The names of these files are application specific and are provided in channel data file.

The cross-section data file RIVflow_xs_data.txt contains the major input information for the river flow model. This file is assembled to contain elevation vs. top width information at each user-specified cross-section along the channel network. The top width information is further classified as main channel, left and right floodplain and inactive storage widths. The file also includes elevation dependent Manning’s roughness coefficients as well as the straight and meandering distances of each cross-section to the starting position of each channel within the system.

The channel data file RIVflow_channel_data.txt includes one line of information specific to each channel within the network. For single channel systems, this file contains a single line.
of data. The data file contains the name, first and last cross-section number and order of the channel. It also specifies the types of boundary conditions at both ends of the particular channel as well as the names of the input files associated with these boundary condition types. The junction data file RIVflow_junction_data.txt contains one line of information for each junction within the channel network. This file is not used for single channel systems. For all networks, this file specifies the total number of inflowing channels to the particular junction and their channel identification numbers. In addition, the file also contains the identification number of the outflowing channel from the particular junction.

The initial conditions along channel are specified in the RIVflow_initial_cond.txt file and contain the initial depth and discharge values observed at each cross-section of the system. These values are used to initiate the simulation and therefore are extremely important for the stability and accuracy of model solutions.

If a channel has an external boundary condition at any end, a boundary condition data file is specified. The names of these files are supplied in the channel data file. It is important to note that only a single channel system would have two boundary conditions at the upstream and downstream ends of the channel. For all networks, a minimum of three boundary conditions are specified both at the upstream nodes of first order channels and the downstream node of the most downstream channel. The files would include the associated data type such as a discharge time series or stage time series or a rating curve as specified the channel data file.

The model also requires a data file if overland flow is present in the system. The small creeks and tributaries could be modeled as overland flow if the reach length that this flow discharges is selected to be small compared to the regular length of a reach. When such a condition is modeled, then the overland flow input file overland_flow.txt must be prepared to include the time-dependent discharge value and the reach number it discharges to.

The data associated with each node in the two dimensional groundwater flow domain is specified in the GWflow_nodes.txt file. This file contains the x- and y- position of the node, the initial hydraulic head elevation prior at starting time of the simulation and the top elevation of the bottom impervious layer. Similarly, the data associated with each quadrilateral element of the two dimensional groundwater flow domain is specified in the GWflow_elements.txt file. This file contains the nodal connectivity of the element as well as the specified yield, hydraulic conductivity and angle of inclination between the global and the principle coordinate systems. The infiltration rate acting on each element of the domain is specified in the GWflow_infilt.txt file as a function of time.

The river/aquifer interface data is provided in the GWflow_lines.txt file. This file includes the connectivity of the nodes in river and groundwater flow domains. It also contains the river bottom sediment hydraulic conductivity and thickness information together with the initial values of average river stage in the corresponding reaches of the channel network. The data associated with any discharge or recharge well in the aquifer is specified in the
The $GWflow\_wells.txt$ file. This file contains the node value of the well as well as the time-dependent flow rate value of the well.

The three types of boundary conditions of the groundwater flow domain are specified in the files $GWflow\_bc1.txt$, $GWflow\_bc2.txt$ and $GWflow\_bc3.txt$. In the first type boundary condition file, the nodal value and the associated time-dependent specified hydraulic head are provided in the data file. In the second type boundary condition file, the two nodes of the boundary side on which the condition applies are given together with the time-dependent specified flux value. Finally, in the third type boundary condition, the two nodes of the boundary side on which the head-dependent boundary condition applies are given with the hydraulic conductivity of the interface as well as the thickness, wetted perimeter, bottom elevation and time-dependent external head value.

The data files associated with the transport models are very similar to their flow counter parts. In the $RIVtrans\_parameters.txt$ and $GWtrans\_parameters.txt$ files, the same discretization related parameters are repeated in addition to some global constants such as the biochemical and radioactive decay coefficients in channel and groundwater flow domains. In addition, the groundwater parameters file also includes the molecular diffusion coefficient.

The $RIVtrans\_channel\_data.txt$ and $RIVtrans\_initial\_cond.txt$ files contain channel specific connectivity data as well as the types of boundary conditions at both ends of the particular channel with the names of the input files associated with these boundary condition types and the initial contaminant concentration values at each cross-section of the channel network.

The model also requires a data file if any overland inflow is present in the system. The small creeks and tributaries carrying contaminants could be modeled as overland flow if the reach length that this flow discharges is selected to be small compared to the regular length of a reach. When such a condition is modeled, then the contaminant concentration in the overland flow is input in the file $overland\_conc.txt$. In addition to the time-dependent contaminant concentration value, the file also contains the reach number it discharges. It is important to note that this file is only prepared for overland inflow to the channel. For overland outflow from the channel, the concentration is fixed and is equal to the river concentration and hence does not require an input file.

The $GWtrans\_nodes.txt$ data file contains the initial contaminant concentration values at all nodes of the groundwater domain. The $GWtrans\_elements.txt$ data file includes the longitudinal and transverse dispersivity values, the density and porosity of the soil matrix as well as the portioning coefficient within the element. The contaminant concentration in the infiltration water is specified in the $GWtrans\_infil.txt$ file for each element of the domain as a function of time.

At the river/aquifer interface, the vertical dispersivity and the porosity of the river sediments are provided in the $GWtrans\_lines.txt$ file. It also contains the initial values of
average contaminant concentration in river at the corresponding reaches of the channel network. The data associated with any discharge or recharge well in the aquifer is specified in the *GWtrans_wells.txt* file. This file contains the node value of the well as well as the time-dependent contaminant concentration value of the recharging well.

The two types of boundary conditions of the groundwater transport are specified in the files *GWtrans_bc1.txt* and *GWtrans_bc2.txt*. In the first type boundary condition file, the nodal value and the associated time-dependent specified concentration are provided in the data file. In the second type boundary condition file, the two nodes of the boundary side, on which the condition applies, are given together with the time-dependent specified mass flux value.

5.2. **General Description of the Lower Altamaha Watershed and Project Area**

The greater Altamaha river basin is the largest watershed in the State of Georgia draining about 25% of the state area. It is also the third largest basin draining to the Atlantic Ocean. It is formed by the confluence of Ocmulgee, Oconee and Ohoopee rivers (Figure 5.1). From the confluence point of Ocmulgee and Oconee rivers down to the Atlantic Ocean, the river system is known as the Altamaha river. It is only this most downstream part of this large basin, which is referred as the Lower Altamaha watershed. This particular application of the coupled flow and transport model focuses on this lower section of the entire Altamaha basin including portions of the Altamaha and Ohoopee rivers as shown in Figure 5.1.

The lower Altamaha watershed has a drainage area of about 3900 square kilometers compared to the total 35200 square kilometers of the entire Altamaha basin. The project area, on the other hand, covers an area of about 2500 square kilometers, which roughly corresponds to 64% of the lower Altamaha watershed. Looking at the overall hypsographic features of the entire Altamaha basin, it can be seen that, with an average width of 26 kilometers, the Lower Altamaha basin is like an 'outflow pipe' or a 'conduit' discharging the combined flows of Ocmulgee and Oconee rivers with some contribution from its own drainage area (Figure 5.1). The basin has an average elevation of 50m and an average annual precipitation of approximately 115cm. At the U.S. Geological Survey gaging station located at Doctortown, GA, the long term mean annual flow of the Altamaha river is measured to be about 400 cubic meters per second.

The lower Altamaha watershed shows all characteristics of typical lowlands with gentle slopes. The maximum elevation difference between the lowest and highest points of the watershed is approximately 90m representing a very mild topography. The main features of the drainage network show a gently meandering pattern in this low land area with a relatively mild slope. This pattern is reflected in Altamaha river with an average slope of 0.0002 m/m below the confluence point of Ocmulgee and Oconee to Doctortown, GA.
Wetlands are commonly observed in the low gradient areas, especially along the river banks and in the coastal region. The contour map of the Lower Altamaha watershed illustrates three distinct topographic zones: (i) the (relatively) highlands; (ii) the transition zone, and (iii) the lowlands or the coastal plains. The topography of the region also shows the gradual increase in floodplain width as river flows towards the lowland zone. Although Altamaha river is the main drainage feature of the lower Altamaha watershed, the drainage pattern becomes extremely complex particularly in the coastal plains downstream of Jesup, GA. In this particular section, Altamaha river does not have a significant drainage area but rather resembles a 'conduit' composed of several inter-connected channels to convey the combined flows of Ocmulgee, Oconee and Ohoopee.

The project area covers a portion of the lower Altamaha watershed drainage area bounded by the U.S. Geological Survey stream gaging stations located at Baxley, Reidsville and Doctortown (Figure 5.2). The drainage pattern in this region is governed by Altamaha river which is later confluenced by Ohoopee river about midway between Baxley and Jesup. The sections of the Altamaha-Ohoopee river system within this area have a total reach length of about 90 km within a sinuous channel of about 115 km.
Figure 5.2. Discretized map of the project area in lower Altamaha river basin
To implement the proposed flow and transport model, this area is discretized by 6,828 quadrilateral finite elements giving a total of 7,031 nodal points. The average element side length along the river sections varies from 150 m to 400 m and about 1000 m elsewhere. On the other hand, the river network that is formed by three channels (i.e., the upstream channel of Altamaha river before the Ohoopee confluence, the Ohoopee river channel and the downstream channel of Altamaha after the Ohoopee confluence) and a single junction is discretized by 391 river reaches giving a total of 394 nodal points. The discretized modeling domain for the proposed model is shown in Figure 5.2.

The channel network is discretized by 394 cross-sections. The required data at these nodes are obtained by using: (i) the measurements taken at three gaging stations by USGS; (ii) the profiles of highway bridges along the river channels; and, (iii) the topographic maps of the area. For all intermediate nodes where no specific feature is present to aid the collect the cross-section data, linear interpolation is performed between the nearest upstream and downstream cross-section with specific data. The top widths are then verified with map readings for consistency. For this particular application, each cross-section is described with 10 sets of elevation-top width pairs starting with thalweg elevation and bottom width of the river.

The Manning’s roughness coefficients are generally considered to be the calibration parameter for channel flow models. Following a series of test runs on the Altamaha river system, a range of Manning’s roughness coefficients are used in the simulations. These values varied between 0.020 to 0.030 within the main channel and 0.030 to 0.070 along the floodplain. Considering the accuracy of the timing of the flood peaks, these values are considered to be very close to the actual roughness values in the river. Unless actual field measurements are obtained, these values could be used as general figures in flood routing simulations in Altamaha and Ohoopee rivers.

Three boundary conditions are specified for the channel flow model. The upstream nodes of the upper channel of Altamaha as well as the Ohoopee river is modeled with a discharge time-series that are obtained from the Baxley and Reidsville river gaging stations operated by the U.S. Geological Survey as shown in Figure 5.2. At the most downstream point of the network, a depth-discharge rating curve is used as the boundary condition. This rating curve is obtained from the Doctortown gaging station (Figure 5.2). The rating curve is generated by the U.S. Geological Survey staff for use in their modeling studies and is given in Figure 5.3.

The initial discharge and stage conditions in the river network are determined by running the model for sufficiently long periods of time with time invariant constant boundary conditions. This method of obtaining the initial conditions is well-defined and documented in the literature (Fread, 1985). As river hydraulics is extremely dynamic compared to groundwater hydraulics, the initial conditions smooth out very rapidly with the real-time boundary conditions imposed on the system. Therefore, any possible errors in the initial conditions quickly fade away and the model returns to accurate real-time operation. On the other hand, the initial conditions are very crucial on the stability of the model in the early
phases of the simulation such that they should still be as accurate as possible to provide a stable start-up.

An unconfined surfacial aquifer overlying the Upper Floridian aquifer is considered to be present in the entire project area, with an average thickness of about 40 m. The groundwater flow domain is assumed to follow the surface drainage boundary line. Hence, the watershed boundary is also believed to be to a flux boundary for the groundwater flow domain. While this assumption may not be true for deep aquifers, it is generally accepted that surfacial aquifers demonstrate a replica of the surface topography. With this consideration, the groundwater flow domain is discretized by 6,828 quadrilateral finite elements and 7,031 nodal points as shown in Figure 5.2.

The soil types in the aquifer were determined using the State Soils Geographic Database (STATSGO) of Georgia developed by the U.S. Department of Agriculture (STATSGO, 1998). Accordingly, the surfacial aquifer consists primarily of unconsolidated, well sorted sand and silt soils. The spatially distributed soil map of the project area is presented in Figure 5.4. The saturated hydraulic conductivities of these soils are assumed to follow the statistically averaged values provided by Carsel and Parrish (1988). The conductivity values used in the proposed model were selected to be 1.25E-6m/s for silt loam soils, 4.05E-5m/s for loamy sand soils and 1.23E-5 m/s for sandy loam soils. In addition, a 0.3m thickness of river sediments is considered to be uniformly present along the channel system with a hydraulic conductivity of 6.94E-7m/s, representing silt material deposited in channel bottoms.

![Figure 5.3. Rating curve at Doctortown gaging station](image)
The Altamaha river system is modeled as a head-dependent line source that creates lateral in/out flow to/from the groundwater flow domain according to the relative values of the river stage and groundwater head. The natural and artificial lakes and ponds in the basin are modeled as constant-head boundary conditions. Moreover, the external watershed boundary is simulated as a no-flux boundary condition except for the immediate vicinity of the Altamaha River near Doctortown gage that is mostly characterized as marshland and modeled as a constant head boundary condition.

The initial conditions in the aquifer is simulated by running the model for extended periods of time with time invariant boundary conditions as well as steady state conditions in the river system since there exists no hydraulic head measurements in the surface aquifer that could serve as initial values of simulations. Considering the strong dynamic link of the aquifer with the surface water features (i.e., primarily the Altamaha river system), this technique of obtaining initial hydraulic head distribution is deemed sufficient.

The overland flow contributions to the model are obtained from the simulation results of an empirical model i.e., the Hydrologic Simulation Program-Fortran (HSPF). The HSPF is
also used to simulate the hydrology of the project area and the overland flow generation scheme of this model is used to obtain the flow of several small creeks and tributaries discharging to Altamaha and Ohooppee rivers (Valenzuela and Aral, 2004). The discharge hydrographs of these overland flow contributions are supplied to the model as approximate figures and is not expected to represent the real overland flow discharges. However, the simulation results are shown to get better even with these approximate results and is, therefore, included in the analysis. It is believed that once an accurate and physics-based overland flow algorithm is derived for large scale applications, the results of the analysis would probably improve to a greater extent.

The simulations are performed over two different time periods. The first phase covers a three-year period starting with 01/01/1988 through 31/12/1990. The second phase, on the other hand, covers a four-year period starting with 01/01/1991 through 12/31/1994. While the first phase is used as the calibration period, the second is used as a verification period. In all calibration and verification simulations, a maximum time step of 86400secs is used to run the coupled flow model. The minimum time step below which the model is coded to stop simulations is selected to be 1secs for this particular application. All simulations initially started with a time step value of 86400secs, which is later modified dynamically within the simulation according to the convergence requirements of the channel flow model as well the number of iterations performed to converge. Commonly the model experiences a wide range of time steps during a simulation depending on the characteristics of the boundary conditions and the flood wave in the channel. The groundwater flow model generally did not impose any limits on the time step due to the relatively slow response times in aquifers. In this regard, the coupled flow model is limited by the time step requirements of the channel flow model. The simulations are performed on an Intel Pentium IV computer with a clock time of 2.4GHz and 1.0GB RAM. The Altamaha river simulations take about 5secs per iteration. On the other hand, the number of iterations per time step and the value of the time step are highly variable and are a strong function of the flood wave that is routed in the channel as well as the boundary conditions.

5.3. Coupled Flow Simulation

The proposed model is used to simulate the flow conditions in the project area shown in Figure 5.2. Two different sets of runs are performed for calibration and verification purposes. The model calibration and verification is performed with respect to the Doctortown gaging station at the most downstream point of the domain (Figure 5.2). Although more than one calibration point would generally provide a better assessment of the simulation results, the data availability in the Altamaha system imposes a single point calibration. In this regard, a midstream calibration point would have been a better option for calibrating the results. Nevertheless, the level of accuracy comparisons with a single calibration point is still believed to provide high standards when particularly in data scarce conditions such as the Altamaha river basin. The simulated vs. observed values of the three-year long calibration period is given in Figure 5.5.
Figure 5.5. Observed vs. simulated results in the calibration period (01/01/1988 – 12/31/1990)

As seen from the figure, the proposed coupled flow provides very good results when compared to the observed values at the Doctortown gage. However, the results are further divided into three separate years to show detailed comparison and to reduce the effect of time scale on the presented graph. These results are shown in figures 5.6a, 5.6b and 5.6c for years 1988, 1989 and 1990, respectively. The detailed comparisons further verify the high level of accuracy achieved by the model. Both timing and magnitude of the flood waves are properly captured. Slight deviations are observed at the peak values which are known to be high flow periods. During these extreme events, the overland flow discharges from the small creeks and tributaries reach to considerable levels that would influence the simulation results. During these periods, a more sophisticated overland flow module is necessary to fully capture the flood peak values. It is clear that, in such high flow periods, the watershed becomes a critical contributor to the river flow in the system as opposed to the general boundary condition driven nature of the system. Therefore, it is possible to conclude that with an accurate overland flow algorithm or with measured discharge data of these creeks and tributaries, one could achieve an almost perfect fit using the proposed model.
Figure 5.6. Observed vs. simulated results in (a) 1988, (b) 1989 and (c) 1990
Unfortunately there exist no measurements to verify the spatial distribution of discharge and/or depth along the channel network. Nevertheless, the discharge distribution along the main Altamaha river is presented in figures 5.7a and 5.7b, representing a low and high flow periods, respectively. It is clearly seen from this figure that, there are small increases in the channel discharge due to overland flow contributions from the tributaries. The spike at the mid-channel is the point where Ohoopee river confluences the Altamaha river.

The response of the groundwater to the dynamic hydrologic and hydraulic variations in river channels could be analyzed by focusing on some of the groundwater nodes in the immediate vicinity of the channel network. The lateral seepage to/from the river in these sections determines the hydraulic head distribution in these areas of the surficial aquifer. This analysis would also help to understand the significance of bank storage on flood peak attenuation in the Altamaha river system. The temporal variation of lateral seepage between cross-sections 45 and 46 in the upstream channel of Altamaha river is shown in Figure 5.8. The figure also presents the discharge hydrograph at cross-section 46. The correlation between lateral seepage and channel discharge conditions is particularly obvious when a major flood event occurs after a relatively steady flow period. In this regard, one could observe the significant lateral outflux from the channel around 9/10/88. When the flood wave arrives, it disturbs equilibrium that was achieved in the relatively steady flow period that covers a couple of months before the event. As a result of the flood event, the stage in the channel increases and creates a lateral outflow from the channel.
Figure 5.7. Spatial distribution of discharge along the Altamaha river
(a) 12/31/1988 and (b) 03/31/1990
Figure 5.8. Temporal variations in lateral seepage and its correlation with channel flow at Node-46 in upstream channel of Altamaha river.
The lateral seepage responses could also be seen in the early parts of the year when consecutive floods arrive to the particular location. However, these interactions are not as clear as the event in September 1988 as the interactions are very dynamic and strongly effected from the earlier events. The model could also predict the impact of bank storage on flood attenuation. Laterally seeping waters from the river are temporarily stored in the immediate vicinity of the channel and is released back to the channel when flood wave passes and river waters recede.

Finally, the groundwater distribution in the watershed is demonstrated in Figure 5.9. The hydraulic head distribution in the figure corresponds to the data at the end of 1988. Since the groundwater flow domain does not experience major changes, a temporal variation in hydraulic head distribution is not meaningful to present. Only in the vicinity of the river channels, the hydraulic head distribution in the aquifer shows variation in accordance with the dynamic link with the river hydraulics.

Figure 5.9. Hydraulic head distribution in the watershed at 12/31/1988
Following the calibration runs, a verification run is also performed to validate the proposed coupled flow model. The verification period covers a four-year period between 1991 and 1995. The simulated vs. observed values of the verification period is given in Figure 5.10. As can be seen from the figure, the model performs accurately in the verification run as well. The flood wave is properly routed in the channel system. The discrepancies between observed and simulated extreme events are still visible in the verification run. Considering relatively insignificant, directionally variable contributions of groundwater seepage, these discrepancies are mainly attributed to the lack of an accurate overland flow simulator. The contribution of overland flow becomes particularly important in extreme events where even small tributaries could carry large discharges.

As seen from the figure, the proposed coupled flow provides very good results in the verification period as well. The results are further divided into four years to show detailed comparison and to reduce the effect of time scale on the presented graph. These results are shown in figures 5.11a, 5.11b, 5.11c and 5.11d for years 1991, 1992, 1993 and 1994, respectively. The detailed comparisons also demonstrate the high level of accuracy achieved by the model. The discrepancies between observed and simulated peak flows are still present in the verification period and are most likely associated with significant overland inflow to the channel from tributaries. Finally, the hydraulic head distribution in the watershed is shown in Figure 5.12 which corresponds to the data at the end of 1991.

![Figure 5.10. Observed vs. simulated results in the verification period (01/01/1991 – 12/31/1994)]
Figure 5.11. Observed vs. simulated results in (a) 1991, (b) 1992, (c) 1993 and (d) 1994
Figure 5.11 (cont’d).
Overall, one could conclude that the coupled surface/subsurface flow model performs satisfactorily. About 4-8% of peak flows are missed at the most downstream location of the watershed where the calibration and verification is made. This discrepancy is expected to be lower in any intermediate point within the system. Nevertheless, this level of closeness is deemed to be normal for a large scale modeling effort such as the one discussed here. It is further believed that these discrepancies are mainly attributed to the relatively inaccurate overland flow discharge values used in this study that are obtained from an empirical model. Once proper mathematical formulation and cost-effective numerical simulation of overland flow is achieved (i.e., in a similar format shown in second coupled model in Chapter 3), the large-scale watershed modeling efforts would most likely yield better results.
5.4. Coupled Contaminant Transport Simulation

The coupled contaminant transport model is applied in the lower Altamaha river basin. Since there are no water quality measurements in the project area, the model is primarily operated as a general tool to understand the overland contaminant transport patterns inside the system with particular focus on the interactions between the river network and the surfacial aquifer. The contaminant transport equations presented herein are all based on the calibrated and verified flow simulations presented in Section 5.3. Therefore, it is believed that the transport simulations would provide valuable insight to the general distribution of contaminants within the watershed. Furthermore, various scenario conditions could be tested with the proposed model and potential vulnerable points to contamination could be determined to assist the watershed management processes. In this regard, the results from the current Altamaha application of the transport model must be viewed from a general perspective and the focus should be on a broad understanding of system characteristics rather than on specific numerical values.

Two important contamination scenarios are analyzed in this section. In the first scenario, the contamination is assumed to initiate from the river system. In this context, the upstream Altamaha river channel is assumed to receive a constant 100mg/L conservative contaminant continuously. The Ohoopee river channel, on the other hand, is considered to be uncontaminated throughout the simulation. The initial conditions in both the river network and the aquifer are taken to be zero. In the second scenario, the contamination is assumed to initiate from the surfacial aquifer at a point close to the Ohoopee river channel. The contaminant area is assumed to sustain 100,000mg/L representing a continuously leaking source. The river system and the rest of the aquifer are considered to be clean and free of any contamination.

These two conditions are simulated with the flow solution of the first 2 months of 1988. The selection of the simulation period was arbitrary since any reasonably long period would cover all possible hydrologic interaction conditions (i.e., river system recharging the aquifer or aquifer discharging to the river system) along the river network. With this simulation period and with the above mentioned two scenarios, it is possible to analyze the influence of contaminated river waters on aquifer water quality and the influence of contaminated aquifer waters on river water quality.

In the first scenario, the contamination is assumed to be entering the system from the upstream boundary of the domain at Baxley gaging station. The analysis of this contaminant is studied in two phases. The first phase covers the first 1-2 days of the simulation during which the contaminant advects and disperses within the channel network until a steady state is reached and the contaminant distribution stabilizes in the network. During this first phase, contaminant does not start to significantly affect the aquifer due to the relatively small response time the groundwater system. On the other hand, the second phase covers the entire extended simulation period where the major focus is on the dynamic interactions of contaminated waters between surface and subsurface systems.
The time-dependent migration of the contaminant is the channel network is shown in Figure 5.13. As can be seen from the figure, the contamination enters the otherwise clean system as a step function, which by itself is a numerically difficult problem to solve. It is then advected and dispersed in the system. The dilution effects of the Ohoopee waters are clearly seen from the figure. The influence of the clean overland flow contributions are not observed as strictly as the Ohoopee river due to the relatively small discharges these tributaries carry as opposed to the main Altamaha river discharge at any particular instant in time. By the end of the second day of simulation, the contamination essentially covers the entire Altamaha river network except for most part of Ohoopee channel that does not receive any contaminant from upstream. Under the hydrologic conditions of this period, the contaminant concentration in the downstream Altamaha channel stabilizes around 94mg/L.

After the initial phase in which the river contaminant concentration stabilizes throughout the channel network, the focus is switched to the contaminant migration in the aquifer. This second phase of the simulation demonstrates the difficulties associated with time scale differences in coupled contaminant transport modeling of the surface and subsurface processes. While the surface contaminant transport is a rapid phenomenon as seen from the first phase of the simulation, the subsurface response is fairly slow and requires longer times for representative output. In this regard, coupled simulation of these two processes necessitates significant computer time. A particular reason for this drawback is the explicit algorithm required to handle the problematic advection operator in the channel transport model as discussed in Chapter 4.

Based on the above discussion, one could conclude that coupled surface/subsurface contaminant transport modeling would become much more feasible when sufficiently accurate implicit algorithms are found to handle the advection related numerical problems. Nevertheless, coupled contaminant transport simulations are still doable in the current form of the model given enough computational time.

In the second phase, the river contaminant concentrations are spatially and temporarily variable only as a function of the Ohoopee river and overland flow discharges. With their zero-concentration values, Ohoopee and tributary flows act as dilution mechanisms to the contaminant in main Altamaha channels (i.e., upstream and downstream). Therefore, the temporal concentration variations are the only major fluctuations observed within the system in response to time-dependent discharge values in these streams. However, these fluctuations are not significant considering their relatively small magnitudes. It is thus possible to conclude that the system operates on a quasi-steady state as long as the specified concentration boundary condition is continuously enforced on the upstream end. Furthermore, the time scales in channel domain are much smaller than their groundwater counterparts such that possible slight variations in channel concentrations do not create long enough changes that could in turn affect the groundwater concentrations. The aquifer contaminant concentration distributions at the end of the first and second months are shown in figures 5.14 and 5.15. It is clearly seen from the figures that both the spatial extent of the contaminated zone as well as the strength of contaminant concentration in these locales increased due to longer exposure to contaminated river waters.
Figure 5.13. Time dependent migration of contamination in Altamaha river network
In the second scenario, the contaminant is introduced to the aquifer at a position that is likely to reach the river network. The selected locale is one of the several alternatives that experiences highest Darcy velocities. The selected area is located in the vicinity of the Ohoopee river roughly at the midstream position between the Reidsville gaging station and the Altamaha confluence point. The contaminated zone covers an area of about 0.2km$^2$ in the Ohoopee flood plain and is about 150m away from the river channel as shown in Figure 5.16.

It is assumed that this area is contaminated with 100,000mg/L of a conservative contaminant. The source zone is selected to be a continuous zone to demonstrate the long term consequences of contamination in the river network and other portions of the aquifer. The contaminated zone is deliberately selected close to the river channel and in an area governed by high groundwater flow velocities towards the river such that the contaminant would quickly reach the river. In this regard, it only takes about 15 days for the aquifer concentration to reach a value of 1000mg/L underneath the river channel as a result of large groundwater flow velocities as well as high dispersion coefficient (i.e., a dispersivity value of 50m is used in the simulations).
The contaminant concentration at the end of one month of simulation in the immediate vicinity of the source area is presented in Figure 5.17. As seen from the figure, the contaminant reaches to significant concentrations underneath the river that works as a significant source for the river pollution under suitable hydrologic conditions.

As the concentration in the aquifer below the river increases, the dispersive flux between the aquifer and river increases since the river is feeding contaminant free waters from the upstream boundary. The lateral seepage towards the river also facilitates the migration of the contaminant to the Ohoopee channel. It is important to note that the mass flux in the lateral seepage is a direct function of the direction of the seepage flux. Hence, the contamination affects the river only when the lateral seepage is towards the river. When the river stage increases due to the arrival of a flood wave, the lateral seepage reverses and river starts to feed the aquifer. The time series graph of lateral seepage in the vicinity of the source zone is shown in Figure 5.18. The dynamic nature of the seepage is clearly reflected in the figure. The dips in the figure correspond to sequential flood waves that enter the reach as shown in Figure 5.19. Consequently, the increased river stage creates a seepage outflux from the river. The timing of seepage outflux dips are directly correlated with the
arrival of the flood peaks. Once the wave is passed the reach, the river stage retreats and seepage is reversed.

In accordance to the above correlation between lateral seepage and river hydrology, the influence of contaminated aquifer water over the river is an intermittent phenomenon. Once the flood wave passes, the river stage retreats, seepage and corresponding advective contaminant transport is reversed. Despite this dynamic behavior of advective flux, the dispersive flux continuously transfers from the high concentration domain (i.e., the aquifer) to the low concentration domain (i.e., the river) and creates a general transport trend independent of the hydrologic conditions of the system. It is important to note however that the magnitude of mass transported with dispersion is small compared to mass transported with advection (i.e., lateral seepage).

Another consequence of the variable lateral seepage direction is a highly variable contaminant concentration within the river. Since the main source of river contamination is lateral seepage-dependent-mass flux (i.e., due to pristine upstream conditions in the river), the river concentration downstream also shows dynamic variations as a direct result of both seepage and upstream discharge variability. The river concentrations downstream the contaminated area is shown in Figure 5.20. The seepage-dependent intermittent behavior of concentration is clearly observed in this figure.

Once the contaminant reaches the river, it is quickly transported downstream. Since the source is next to the Ohoopee river and the upstream Altamaha channel is clean, significant amount dilution occurs at the Ohoopee-Altamaha junction. The Ohoopee channel concentrations are significantly diluted with pristine Altamaha waters and continue their downstream transport. The lateral seepage along the downstream Altamaha channel allows the re-introduction of contaminated waters back to the aquifer. Therefore, the river system acts as a conduit for fast transport of contaminants. The contaminant distribution within the aquifer after one and two months of simulation are shown in figures 5.21 and 5.22. As can be seen from the figures, the contaminant is slowly entering the otherwise clean aquifer downstream of the contamination zone. It is clearly seen that the contamination is limited to the immediate vicinity of the river channels. Any further migration towards the inner regions of the aquifer did not occur in these time periods as the general groundwater flow direction is mostly directed towards the main river network in the watershed. Only during flood events, intermittent flow reversals allow rapid contaminant transport towards the inner regions of the aquifer. In all other hydrologic conditions, the magnitude of dispersive flux, which is independent of the dynamic hydrology of the system, is not deemed to be sufficient to create extensive migration of contaminants to such inner regions of the aquifer. Therefore, it can be concluded that depending on the hydrology of Altamaha system, the contamination in the river might migrate large distance inside the aquifer particularly for extremely wet years that are characterized by the river system feeding the surfacial aquifer.
Figure 5.16. Contaminated zone location in Scenario-2
Figure 5.17. Contaminant concentration in the immediate vicinity of the source area after 1 month of simulation.
Figure 5.18. Lateral seepage near the contamination zone

Figure 5.19. Discharge in the reach near the contamination zone
Figure 5.20. Contaminant concentration in the river at the contaminated zone
Figure 5.21. Aquifer contamination after 1 month of simulation
Figure 5.22. Aquifer contamination after 2 month of simulation
6. Conclusions and Recommendations

6.1. Conclusions

Large scale watershed modeling has long been an important challenge for the hydrologist. Numerous models have been developed to analyze possible flow patterns over a watershed in response to some precipitation event. Although most of these models used empirically-based lumped parameter formulations by neglecting or oversimplifying the underlying physical processes, they have served their purpose and provided basic data without going through a detailed analysis. In recent years, the trend has switched to a more fundamental understanding of the processes affecting the overall response of the watershed and hydrologic modelers have directed their focus on physically-based distributed parameter models. These models are based on rigorous mathematical formulations of physics laws defining the flow of water over a watershed and provide a better understanding to the watershed processes. Nevertheless, their application to large scale watersheds is severely limited with respect to computational power requirements. Mainly due to the distributed nature of these models and the numerical solution techniques implemented to capture the flow patterns, these models require fine discretizations, which in turn increase the overall matrix size that need to be solved in each computational time step. Therefore, both computational speed and memory requirements could easily become unmanageable given the limits of today’s computers. A perfect example to such limitations is the overland flow domain. Due to its spatially and temporally discontinuous flow pattern, very small water depths as well as strong non-linearity associated with land characteristics, overland flow models require finer spatial and temporal discretization. Furthermore, the flow boundaries are not as well-defined as the other processes such as the channel flow or groundwater flow. Another example to limitations with respect to computational speed and memory requirements is the groundwater flow in the unsaturated zone. The moisture movement in this zone is strongly non-linear due to the dependency of hydraulic conductivity and pressure head on moisture content. Effectively capturing this dependency requires fine discretization which becomes a problem in large scale watershed models.

Considering the limitations mentioned above, this study is an attempt to blend the powerful distributed parameter models with relatively simple lumped parameter models to form a so-called hybrid model that could solve the major flow pathways in a distributed sense and simplify others in a lumped format. In this regard, the proposed hybrid model considers the channel flow and groundwater flow as major pathways and treats them in a fully distributed sense using physically based formulations. The proposed model also implements full coupling of these flow processes along the river bed using lateral seepage. The model, on the other hand, considers the overland flow and unsaturated zone flow in a lumped parameter fashion without going through the details of these processes in a distributed modeling sense.

When watershed processes are analyzed in an integrated fashion, coupling becomes a major issue. Coupling provides the link between different flow pathways and maintains the
continuity of the system. Although as essential as it is, coupling is a computationally costly procedure where the common parameters are generally iteratively improved until convergence is achieved with respect to a pre-determined criterion. Previous studies implemented iterative algorithms, which became a standard procedure to couple flow pathways. In this study, a new simultaneous solution procedure is proposed to couple surface and subsurface flow along the river bed via the lateral seepage flow. The new technique does not rely on iterative improvement that makes it a faster procedure as opposed to the iterative technique. The method is based on the principle of solving channel flow and groundwater flow equations within a single matrix structure considering the interacting terms within the equations. Although the method requires the solution of larger matrices, it is still faster and more accurate than the alternative methods available. As the two systems are essentially solved together at once, it is also a more physically realistic technique to handle inter-pathway interactions of hydrologic cycle.

This study is also believed to be one of the earliest examples of coupled contaminant transport modeling. A coupled surface-subsurface contaminant transport model is formulated to provide a basic understanding for contaminant transfers between interacting domains. The proposed transport model uses the coupled flow solution and implements an advective-dispersive mass transport function along the river bed. This coupled analysis of contaminant transport is thought to be an important mechanism for strongly interacting systems under suitable hydrological conditions. The numerical difficulties associated with the advection operator in channel transport model hinder the use of the proposed simultaneous solution algorithm. As an explicit solution procedure is necessary to capture the behavior of contaminants in advection dominant systems, an operator splitting algorithm is implemented to separate the explicit advection from the remaining operators. Although this numerical separation scheme appears to violate the simultaneous presence of two physical transport processes, it is mathematically sound and essential for accurate analysis of transport in advection dominant systems. In this regard, the proposed simultaneous solution algorithm is modified such that the advection operator is solved discretely before the dispersion, and remaining operators are solved simultaneously with the groundwater transport equation in a single matrix structure. Because of this change, the transport solution algorithm is called the semi-simultaneous solution method. The method could, however, be made fully simultaneous without much difficulty when an implicit advection algorithm is developed that would numerically yield accurate results without the restrictions of its explicit counterpart.

The proposed coupled flow and transport models are applied to the lower Altamaha watershed in southern Georgia. Long term flow and contaminant transport simulations are performed to analyze the hydrologic and geo-hydrologic characteristics of the watershed. The coupled flow simulations revealed a dynamic and spatially variable interaction pattern between the river and the surficial unconfined aquifer. Seepage rates are found to be a strong function of the hydrologic conditions in the river. The results of the flow simulations have shown good match with the observed data obtained from the Doctortown gauging station. The simulated values are also shown to capture the timing and magnitude of observed flood hydrographs accurately. The calibrated flow patterns in the river channels
and in the aquifer are then used to test several contaminant transport scenarios for the watershed. The results from the contaminant transport simulations revealed the fact that contaminated river water is much likely to create more significant consequences over the aquifer than would the contaminated aquifer water over the river due to the significant dilution effect of the river water over the contaminated seepage from the aquifer. Furthermore, it is observed that the immediate vicinity of the river channels is most likely to experience the highest contaminant concentrations under suitable hydrologic conditions due to the slow movement of groundwater. Therefore, any incidental instantaneous spill to the river is not likely to create significant groundwater pollution as the contaminants are quickly washed away with fast flowing river waters. On the other hand, any potential continuous source of contamination near a discharging section of the aquifer (i.e., such as a leaking tank) is likely to create problems in the otherwise clean river waters despite the dilution effect in the river. In this regard, it is believed that the coupled flow and transport model would allow more detailed analysis of possible sources and migration patterns of contamination in the lower Altamaha watershed.

6.2. Recommendations

Although this study provides a unique approach to watershed modeling by introducing the concept of hybrid models, the future of watershed modeling still necessitates using a fully distributed approach in all possible subprocesses of the water cycle. In the future, mathematical representation and numerical solution procedures of these processes would evolve to such a degree that the modeler would not have to compromise the fully physically-based distributed approach. In this regard, the author believes that there would be two major areas of work that the future hydrologic modeler would focus on. While one of these areas would involve better representation of flow pathways with more accurate models, and the other one would focus on development of better numerical techniques for these sophisticated mathematical models.

Without doubt, there is work to be done in better describing the overland flow component. Such an approach must not only represent the temporal discontinuity accurately but also must incorporate it in a suitable format where long term simulations would be possible including the overland flow domain in the overall simulations. It is believed that time-dependent moving boundary analysis and temporal Dirac delta representations would become the hot topics of overland flow modeling in years to come. Better numerical algorithms would then be required to accurately handle the moving boundary problem, small water depths and wetting-drying conditions in the three-dimensional topography of the watershed.

The current state of the proposed model could be improved by incorporating more sophisticated descriptions of subprocesses that would certainly require more computational power and data. For example, a variably-saturated three-dimensional groundwater model would certainly be an improvement of flow processes in porous media. Such an improvement would not only eliminate the one-dimensional representation of the unsaturated zone but also would solve the entire soil column as a whole in a variably-
saturated fashion. The data requirements of such a model would be extremely large compared to the present model and it can only be applied over a very limited spatial domain unless sophisticated data collection and analysis methods are developed and made available to the modeler in an easy to access fashion. In the long run, a two-dimensional river model might be linked to this three-dimensional variably saturated groundwater model. Such an improvement would probably constitute what is called the ‘ultimate watershed model’. However, better coupling mechanisms would then need to be developed before the interactions between the river and the aquifer can be accurately simulated.

It is believed that enhanced numerical algorithms would have to be incorporated into river and groundwater transport models for more accurate results and for more general applicability of the model. Such algorithms would better handle the dual-nature of the advective-dispersive transport equation. However, compromises might need to be made in terms of using such algorithms versus using simultaneous solution technique since such algorithms generally require the use of explicit components to handle the advective transport that, in theory, violate the idea of simultaneous solution. In this regard, high-accuracy implicit schemes are to be developed before a fully simultaneous coupling of surface and subsurface transport processes could be done similar to their flow counterpart.

Further research is also necessary on scale issues of coupled hydrologic modeling. Separate model components with different spatial and temporal scales are difficult to couple dynamically. Particularly, scale issues associated with slow and fast hydrologic processes create problems in terms of computer resources and data availability. Therefore, only after computational speed would reach to a point where the entire watershed hydrology could be modeled with the smallest time scale requirement, one could achieve an ultimate simultaneous coupling of all processes.

An essential part of watershed modeling is the requirement for calibration and verification data. Such data sets are only available for small experimental watersheds. At larger scales, researchers are faced with data insufficiency to calibrate and verify their models. Therefore, additional resources should be allocated to provide not only extensive field studies but also to increase the density of standard data collection facilities that are currently available. These efforts must be geared towards obtaining better subsurface data since surface flow data is comparably more abundant.

Finally, the author firmly believes that, in the long term, the hydrology and hydraulics of watersheds will be modeled as a whole in a fully coupled way using three-dimensional models. Such a comprehensive model would simultaneously couple all processes and would solve them as a single system considering all the interactions between each other without the need to introduce artificially separated flow domains. This study is only an initial step towards such an approach.

A users manual is presented in this section of the report. The assumptions and highlights of the proposed model are discussed. The details associated with input data preparation and output data analysis are given in the following subsections.

7.1. Assumptions and Highlights of the Proposed Model

The proposed model could only run in SI units. Therefore, all data must be converted to suitable SI units to be used in the model.

The channel flow model is currently limited to a maximum of 1000 cross-sections and 25 data lines per cross-section to define the elevation-top width characteristics of these cross-sections. The model could also handle a maximum of 10 channels. Since these parameters define the dimensions of the matrices in the system, the model could not run with larger systems. The source code must be modified to allow simulations of larger systems.

The model is designed to run subcritical flows where the Froude number is below 1 at all cross-sections throughout the simulation. It is possible that certain cross-sections, particularly cross-sections with limited flow area such as bridge crossings, are subject to supercritical flows in high flow periods due to the reduced flow area. When such a condition occurs, the non-linear solver in the model would quickly diverge and eventually crash due to negative flow depths. If such a condition is to occur, the user must check the output and restart the run after the particular high period ends. However, the initial conditions and the data files must then be modified for the new start up period.

Initial conditions of the channel flow are extremely important for a successful start up of the simulations. If the user inputs unrealistic conditions, the model could quickly diverge and crash. The only remedy is a trial and error solution and a slow start with constant boundary conditions until the model stabilizes. The stabilized values could then be used in the actual simulation as initial conditions.

7.2. Input Files and Data Preparation

The proposed flow and transport model requires several input files that are shown in Table 5.1. In this section, a description of the input parameters and their required format will be discussed in details to assist data preparation activities. All model files are presented in the following paragraphs.
• *time_data.txt*

This file contains the main simulation parameters that define the simulation start and end times as well as time step related parameters. A sample *time_data.txt* file is shown in Figure 7.1. This file is a space-delimited file which is organized in two columns. The first column covers the first 25 characters of each line and includes a brief description of the data parameter that follows. The next 10 characters contain the actual data for this parameter. This format should be followed strictly for accurate data input to the model.

![Figure 7.1. “time_data.txt” input file](image)

Following a header line, the starting day, month, year and time of the simulation are input in the consecutive four rows of data. The starting time position is a derived variable that maps each calendar date-time combination to a single number. The frame of reference for this conversion is the date 1/1/1900 00:00am, which corresponds to 1.0. Any time within the 24-hr day corresponds to the fractions of the number. In this manner, all other date-time combination is evaluated easily. For example, 1/1/1988 12:00 pm corresponds to a value of 32143.5. A similar idea is applied for the ending time of the simulation. The user could use the Microsoft Excel to find the time position of any date/time combination.
The next three rows of data specify the general, maximum and minimum time step values to be used in the simulations. The adaptive time stepping algorithm uses a number of simulation-specific information such as the number of iterations required to converge in a particular solution in order to dynamically modify the operational time step value of the simulation. The value ‘dt’ is the initial value of this operational time step value, which can be less than or equal to the maximum allowable value, ‘dt_max’, and bigger than or equal to the minimum allowable value, ‘dt_min’. These minimum and maximum values of the time step set the limits for the time stepping algorithm. The maximum and minimum time step values cannot go beyond the values of 86400 secs and 1 sec, respectively. In this regard, the time step of the simulation experiences a value between 1 and 86400 secs throughout the simulation period. Furthermore, the maximum allowable time step must always be less than or equal to the minimum time step between any time-dependent data such as the upstream discharge hydrograph of river flow model or infiltration values of groundwater flow. Therefore, the model can not step over the time-dependent data values specified in other input files and must always be operated with a time step less than or equal to the minimum of such data.

The ‘omega’ for groundwater model corresponds to the time-weighing coefficient used in the groundwater flow discretization. This model uses a Crank-Nicholson type approximation and this value is always fixed at the value of 0.5. It is left as an input parameter for future modifications of the model. On the other hand, ‘theta’ for river model corresponds to the user-specified time-weighing parameter used in the Preissmann scheme. The value is taken to be between 0.5 and 1.0 for implicit simulations. The ‘alpha’ for river model is used to evaluate the initial guess values of river flow model parameters (i.e., discharge and stage) using the two previous time-line values of these parameters. The alpha value provides a time-weighing between these two time lines in evaluating the values for next iteration and hence must take values between 0.0 and 1.0. However, a value of 0.5 is generally used and is deemed to be accurate for most applications.

Finally, the ‘ite_max’ and ‘ite_min’ parameters set the limits for the adaptive time stepping algorithm beyond which a change in time step occurs. In this regard, when the number of iterations within a time step becomes equal to or exceeds the value specified in ‘ite_max’, then the operational time step is automatically reduced to 75% of its present value. On the contrary, when the number of iterations within a time step becomes equal to or falls below the value specified in ‘ite_min’, then the operational time step is automatically increased to 125% of its present value. In addition to these modifications, the time step value is also automatically halved when a negative depth problem occurs within a particular time step. The model is designed to allow 16 of such halving of the time step due to negative depth problem and stops if a 17th such reduction is required. If such a condition occurs, the user must double-check the accuracy of the cross-sectional data and also make sure that the system does not experience supercritical flow conditions for that particular instant in simulation.
This file contains information on whether contaminant transport will be performed or the current run would only involve a flow simulation. The file also includes the convergence criteria for the transport simulation which is used to check the convergence of the coupled contaminant transport simulation in each time step. A sample `general_data.txt` file is shown in Figure 7.2. As seen from the figure, this file has the same format as the `time_data.txt` file and is a space-delimited file which is organized in two columns. The 25-character wide first column of each line includes a brief description of the data parameter that follows. The next 10 characters contain the actual data for this parameter. This format should be followed strictly for accurate data input to the model.

![Figure 7.2. “general_data.txt” input file](image)

When contaminant transport simulation is to be performed together with the flow simulation, then the parameter is set to 1, else, the parameter is set to 0. The second row data specifies the convergence criteria used in the model to test coupled transport results. It generally takes less than 3 iterations per time step due to the small time steps required by the transport model.
• **RIVflow\_parameters.txt**

This file contains the main simulation parameters that define the flow simulation in river channels. A sample *RIVflow\_parameters.txt* file is shown in Figure 7.3. As seen from the figure, this file has the same format as the ‘time\_data.txt’ file and is a space-delimited file which is organized in two columns. The 25-character wide first column of each line includes a brief description of the data parameter that follows. The next 10 characters contain the actual data for this parameter. This format should be followed strictly for accurate data input to the model.

![Figure 7.3. “RIVflow\_parameters.txt” input file](image)

Following the header line, the number of channels, junctions and cross-sections within the entire channel flow system are input in the file. The number of datalines in cross-section data file is then input in the fourth line. This data specifies the total number of stage-top width combinations that are used to define all cross-sections. It is important to note that the number of data lines must be the same in all cross-sections. Therefore, although a particular cross-section might be relatively simple compared to others in the system and would normally not need as many datalines as another cross-section, this section is also ‘over’ specified to be consistent with other cross-sections of the system. The next data specifies the total number of reaches that receive overland flow.
The number of boundary conditions is then input in the next row. It is important to note that a single channel would always have two boundary conditions i.e., one on each end, whereas a channel network could have different number of boundary conditions depending on the number of channels comprising the network and their configuration. The user must be aware of the fact that the proposed model could only model dendritic (i.e., tree type) networks and would not simulate looped systems. Furthermore, the user must also make sure that this data set is free from any logical errors.

The next data row specifies if the user would input the initial conditions directly or would allow the model to compute initial values from a gradually-varied steady flow simulation of the system. A value of 1 would represent an internal initial condition evaluation and 0 would mean that the user would supply the initial condition data. Since initial condition data is extremely important for the stability and successful start-up of the system, utmost care should be given to the evaluation of initial conditions. Several experiences with different simulation conditions revealed the fact that internal evaluation alone would not be sufficient to supply accurate initial conditions that define the system. The author recommends that an initial test run be made by allowing the model to evaluate the initial conditions internally by setting the value of the parameter to 1. It should however be noted that even this run would require some initial data which could only be supplied with some engineering judgement. A constant water depth at all cross-sections is a good starting point to evaluate the initial conditions. The model would then use this information to internally compute its initial condition values. This would then be used as a first estimate for initial data. The author recommends that the early test runs of a system must be performed with constant boundary data for a sufficiently long period of time within which the system would reach a quasi-steady state. In essence, this technique uses the originally unsteady model to perform steady state simulations. The results of this sufficiently long simulation with constant boundary data would then be used as the initial conditions of the real runs with time-dependent real boundary conditions. This three step procedure is believed to give fairly accurate initial data to start the actual simulations. When the final initial condition data is achieved, the value of the parameter in the input file is set back to 0 to allow the model to read this initial data from the RIVflow_initial_cond.txt data file.

Finally, the tolerance value required for the non-linear solver is input in the last row of this data file. As with all non-linear solvers, small values of the tolerance would mean large number of iterations to converge. Therefore, it is extremely important to select a tolerance value that would result in feasible run times. It should also be noted that using a smaller tolerance would not always create significant changes in the computed results. Moreover, when a smaller tolerance is used, the user must also modify the iteration parameters specified in the time_data.txt file as discussed above.
• *RIVflow_xs_data.txt*

This file contains the cross-section data that defines each node within the finite difference discretization. A portion of *RIVflow_xs_data.txt* file is shown in Figure 7.4. As seen from the figure, this file has a different format than the rest of the files discussed so far. It is also a space-delimited file where cross-sections are separated from each other by empty rows. The first line of each cross-section is a 50-character text line that describes the cross-section. The next line has three data values. The first data is input in a 10-character wide space and corresponds to the cross-section identification number that is used to uniquely characterize a cross-section within the system. The next data is written in 20-character wide space and define the position of the cross-section relative to the first cross-section of the particular channel while traversing from the flood plain. It is also known as the reach length between the particular cross-section and the next one. The third data is also written in a 20-character wide space and define the position of the cross-section relative to the first cross-section of the particular channel while traversing from the channel bed, thus giving the sinuous distance to the starting cross-section.

![RIVflow_xs_data.txt input file](image)

Figure 7.4. A portion of "RIVflow_xs_data.txt" input file

The main cross-section elevation-top width table is then input according to the number of datalines specified in the *RIVflow_parameters.txt* file. In the above figure, each cross-
section is represented with a total of 10 datalines. The data is organized in 7 columns which are 10-character wide. The first five columns are used input the elevation and corresponding channel, left floodplain, right floodplain and dead storage top widths, respectively. The last two columns are reserved for Manning’s roughness coefficients in the channel and in the floodplain. When this information is supplied for all layers, a cross-section is fully defined and required parameters such as the area and total conveyance could be derived easily. It is, however, important to note that the 10-character wide space-delimited format should be followed strictly for accurate data input to the model. Even a slight modification of the width of a field would result in a totally erroneous values read as the cross-section data, which would in turn cause the model to crash.

The model is equipped with several internal checks for the accuracy of the cross-section data. It could detect and warn the user for conditions that violates the requirement that the channel top widths must monotonically increase from bottom to top. Therefore, the model could not handle ‘caving’ within a channel.

- **RIVflow_channel_data.txt**

This file contains the channel data that defines the general overlay of the river network. An example of **RIVflow_channel_data.txt** file is shown in Figure 7.5. As seen from the figure, this file has a different format than the rest of the files discussed so far. It is also a space-delimited file where each channel is input in a separate row

Following a header line, a 5-character wide column stores the channel identification number. The second column stores a channel identification name in a 20-character wide field. The third and fourth columns are both 10-character wide fields and store the starting and ending cross-sections of the channel. In the particular example of Figure 7.5., the Ohoopee channel start with the cross-section 91 and ends with 242. Therefore, a total of 152 cross-sections define the Ohoopee channel. The next column covers a 10-character wide space and is used to specify the Strahler order of the channel. According to this ordering scheme, an upstream channel is always assigned a first order. A second order channel is formed when two first order channels confluence. In this regard, upstream Altamaha and Ohoopee channels are considered to be first order channels for this particular application. The downstream Altamaha channel would then become a second order channel. It is imperative to note that this ordering is a scheme applied for the model-specific discretized system not the actual river network.
Figure 7.5. “RIVflow_channel_data.txt” input file

The next 6 columns define the boundary condition data associated with each channel. Normally, a channel could have a maximum of two boundary conditions only when the system is comprised of a single channel. For all other conditions, channels would have one or no boundary conditions depending on the relative position of the channel within the network. In the example shown in Figure 7.5., the two upstream channels (i.e., Altamaha-1 and Ohoopee) have one upstream boundary condition and the downstream channel (i.e., Altamaha-2) has one downstream boundary condition. The 5-character wide column that immediately follows the channel order is used to input whether a channel would have an upstream boundary condition or not. If an upstream boundary condition is assigned to the particular channel, then the value of this parameter is set to 1. If the channel does not have an upstream boundary condition, the value of this parameter is set to 0. If the channel has an upstream boundary condition, then the next two fields are completed, otherwise they are left empty. The first one of these two columns specifies the type of the boundary condition. The proposed model would allow the use of the following types of upstream boundary conditions:

1. Stage hydrograph
2. Discharge hydrograph
Generally, a discharge hydrograph is commonly used as an upstream boundary condition as shown in Figure 7.5. Regardless of the type of the boundary condition, the name of the boundary condition file must be input in the next column that is a 20-character wide field. Therefore, the file name could not be larger than 20 characters including the extension. A portion of a sample discharge hydrograph boundary condition file is given in Figure 7.6. The file is a tab-delimited file and starts and ends the actual simulation start and end times. Following the header line, the data includes two columns separated with a tab. The first column specifies the position of time and the second column specifies the actual discharge data observed at that time in cubic meters per second. The time step between two data lines is arbitrary but no two consecutive data could be closer than the minimum allowed time step. It is also important to note that a minimum of 4 timelines must be specified in a discharge time series data file, the first and the last of which must be the simulation starting and ending times, respectively. It is important to mention that a similar pattern is used in the data file if a stage hydrograph is used as the boundary condition. In such a case, the actual data values become the water surface elevation reported in meters.

![Figure 7.6. A discharge boundary condition file](image)

The next 5-character wide column that immediately follows the file name of the upstream boundary condition is used to input whether a channel would have a downstream boundary condition or not. If a downstream boundary condition is assigned to the particular channel,
then the value of this parameter is set to 1. If the channel does not have a downstream boundary condition, the value of this parameter is set to 0. If the channel has indeed an downstream boundary condition, then the next two fields are completed, otherwise they are left empty. The first one of these two columns specifies the type of the boundary condition. The proposed model would allow the use of the following types of downstream boundary conditions:

1. Stage hydrograph
2. Discharge hydrograph
3. Single-valued rating curve
4. Looped rating curve
5. Critical flow section
6. Normal depth

The stage hydrograph and the single-valued rating curve are two most commonly applied boundary condition types at the downstream boundary of a channel. The stage and discharge hydrograph have similar file formats as discussed above. The single-valued rating curve data file should always bear the file name `rating_curve.txt` regardless of the application. A sample single-valued rating curve data file is shown in Figure 7.7.

![Figure 7.7. ‘rating_curve.txt’ input file](Image)
The rating curve file is a dual-formatted file. The first row of the file is in space-delimited format and contains two fields. The first field is a 25-character text field that used to store the description of the data contained in the next field. This second field is a 10-character wide space and is used to store the total number of data sets that would be read from the rating curve data file. Immediately following this data, an empty row is placed to separate the following tab-delimited data. The third row of the file contains the header information for the remaining data sets. Finally, the last portion of the data file contains the actual rating curve data organized in a tab delimited format. The first column contains the data set identification number. The second and third columns specify the depth and the associated discharge value observed at the rating curve cross-section. The depth values are reported in meters whereas the discharge data is input in cubic meters per second. It is extremely important that the range of the rating curve covers all the possible discharge values that the cross-section would experience during a particular run. If a discharge that is larger than the maximum discharge value specified in the data set arrive the cross-section at any particular instant in simulation, the model would stop execution. Therefore, it is the user’s responsibility to guarantee that the entire discharge spectrum is covered in the rating curve data file. It also important that the total number of actual data sets in the input file must be consistent with the information specified at the beginning of the file.

The looped rating curve and critical flow section boundary conditions do not require any input file. These boundary conditions are evaluated internally by the model. The normal depth boundary condition, however, requires that a discharge hydrograph is supplied by the user as an input file. The model internally converts the provided discharge data to a normal flow depth and then uses this value as the boundary condition. It must be noted that both these three types and the discharge hydrograph boundary condition are rarely used in channel flow model. Stage hydrograph and the rating curve are the two most common data types for a downstream boundary condition.

- **RIVflow_junction_data.txt**

This file contains the junction specific data. A sample *RIVflow_junction_data.txt* file is shown in Figure 7.8. This file is a space-delimited file and is only required for channel networks which contains at least one junction. This file is not used for single channel systems. In systems with multiple junctions, each junction is input as a separate row of data. The 5-character wide first column is a junction identifier. The 20-character wide second column is used to specify the total number of channels inflowing to the junction. The model allows a maximum of 3 channels inflowing to a single junction. This assumption is deemed sufficient since it is highly unlikely that more than three river channels confluence at a particular point in a watershed.
The following three 5-character wide columns are then used to input the channel identification number that flows into the junction. If there are only two channels flowing into the junction, the third field is left empty as shown in Figure 7.8. Finally, the 20-character wide field contains the outflowing channel’s identification number. Since the model only allows dendritic networks, only a single channel could outflow from a junction. If the system contains more than one junction, then the next junction is input in the next row following the same format.

- **RIVflow_initial_cond.txt**

This file contains the initial condition data to start the simulations. A portion of the sample *RIVflow_initial_cond.txt* file is shown in Figure 7.9. As discussed before, this file could either be supplied by the user or could be created internally by the model. In either case, this file must be a tab-delimited file and must contain three columns of data. In the first column, the cross-section identifier is input. The second and third columns contain the initial depth and discharge values recorded for the cross-section. The depth values are input in meters and discharge values are input in cubic meters per second. The model internally converts the depth data to stage data, which is the unknown variable of the channel flow model.
**GWflow_parameters.txt**

This file contains the main simulation parameters that define the flow simulation in groundwater. A sample `GWflow_parameters.txt` file is shown in Figure 7.10. As seen from the figure, this file has the same format as the `time_data.txt` file and is a space-delimited file which is organized in two columns. The 25-character wide first column of each line includes a brief description of the data parameter that follows. The next 10 characters contain the actual data for this parameter. This format should be followed strictly for accurate data input to the model.

Following the header line, the number of nodes, elements, wells, lines, type-1 boundary conditions, type-2 boundary conditions and type-3 boundary conditions are input in the file. Finally, the tolerance value required for the non-linear solver is input in the last row of this data file. As with all non-linear solvers, small values of the tolerance would mean large number of iterations to converge. Therefore, it is extremely important to select a tolerance value that would result in feasible run times. It should also be noted that using a smaller tolerance would not always create significant changes in the computed results. However, when a smaller tolerance is used, the user must also modify the iteration parameters specified in the ‘time_data.txt’ file as discussed above.
• *GWflow_nodes.txt*

This file contains the nodal data for groundwater flow domain. A portion of the sample *GWflow_nodes.txt* file is shown in Figure 7.11. The file is in tab-delimited format which is organized in five columns. The first column is used to input the nodal identifier. The second and third columns are used to input the x- and y- positions of the node. In the fourth and fifth columns, the user inputs the initial hydraulic head observed at the node and the bottom elevation of the aquifer at the particular node, respectively. As in river flow domain, the initial conditions of the hydraulic head distribution in the aquifer could be obtained by running the model with constant boundary conditions for a sufficiently long period of time.
This file contains the element specific data for groundwater flow domain. A portion of the sample *GWflow_elements.txt* file is shown in Figure 7.12. The file is in tab-delimited format which is organized in nine columns. The first column is used to input the element identifier. The second thru fifth columns are used to input the nodal connectivity data of the element. The sixth column is used to input the specific yield value of the element. In columns seven and eight, the user inputs the hydraulic conductivity values in meters per second along the principle coordinate directions. Finally, the last column is reserved for the angle in degrees that the principle coordinate axis makes with the global coordinate axis for the particular element. The model internally performs a conversion between hydraulic conductivity along the local coordinate axis and the hydraulic conductivity along the global coordinate axis.
Figure 7.12. A portion of ‘GWflow_elements.txt’ input file

- **GWflow_wells.txt**

This file contains the well data for groundwater flow domain. A sample *GWflow_wells.txt* file is shown in Figure 7.13. The file is in tab-delimited format. If the number of wells data value in *GWflow_parameters.txt* file is bigger than zero, the values inside the *GWflow_wells.txt* file is read by the model. Otherwise, it is ignored. In the example shown in Figure 7.13, the domain has 5 wells located at nodes 16, 700, 1328, 3891 and 5010.

Since well flow is a time-dependent input, the file is structured to allow variable values with respect to time. As with the discharge boundary condition files in river flow domain, the input file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. The corresponding flow rates of wells located at nodes 16, 700, 1328, 3891 and 5010 are specified for each timeline. It must be noted that although the flow rate value of a particular well might not change at some particular time level, it must still be included in each time line. Therefore, all time lines of *GWflow_wells.txt* file must include all wells regardless of a change in the flow rate value. In the data file, a positive flow rate corresponds to a discharging well and a negative flow rate corresponds to a recharging well.
• **GWflow_lines.txt**

This file contains the line source specific data for groundwater flow domain. A portion of the sample *GWflow_lines.txt* file is shown in Figure 7.14. The file is in tab-delimited format which is organized in eight columns. The user must be aware of the fact that the river network serves as a line source for the groundwater flow domain. Therefore, this file provides a link between the two flow domains. The first column is used to input the line segment identifier. The second and third columns are used to input the nodal connectivity data of the line segment. The fourth through sixth columns are used to input the hydraulic conductivity and thickness of the river bottom sediments as well as the initial river stage in the line segment, respectively. The last two columns are used to input the river cross-sections that correspond to the groundwater flow nodes given in columns 2 and 3. Therefore, this file provides a mapping between the groundwater flow domain nodal numbering scheme and the river flow domain nodal numbering scheme. It is important to note that the numbering scheme should follow the river flow direction and cross-section numbering. The hydraulic conductivity and the thickness of the bottom sediments are input in meters per second and meters, respectively. The river stage is also given in meters.
This file contains the infiltration/exfiltration data for groundwater flow domain. A portion of the sample *GWflow_infilt.txt* file is shown in Figure 7.15. The file is in tab-delimited format. The file assigns an infiltration/exfiltration value to all elements of the domain regardless of whether the element receives infiltration/exfiltration or not. In the particular example, this file would contain all 6828 elements of the domain. Since infiltration/exfiltration is a time-dependent input, the file is structured to allow variable values with respect to time. As with other time-dependent input files, the input file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. In the data file, a positive rate corresponds to an exfiltration condition and a negative rate corresponds to an infiltration condition. The infiltration/exfiltration rate must have units of meter per second.
This file contains information regarding the type-1 boundary condition in the groundwater flow domain. A portion of the sample `GWflow_bc1.txt` file is shown in Figure 7.16. The file is in tab-delimited format. If the number of type-1 boundary conditions is bigger than zero, the file is read by the model. Otherwise, it is ignored. Since type-1 boundary condition is a time-dependent input, the file is structured to allow variable values with respect to time. As with the discharge boundary condition files in river flow domain, the input file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. It must be noted that although the value of the boundary condition at a particular node might not change at some particular time level, it must still be included in each time line. Therefore, all time lines of `GWflow_bc1.txt` file must include all boundary condition nodes regardless of a change in the nodal hydraulic head value. In the data file, the nodal hydraulic heads are given in meters.
This file contains information regarding the type-2 boundary condition in the groundwater flow domain. A sample *GWflow_bc2.txt* file is shown in Figure 7.17. The file is in tab-delimited format. If the number of type-2 boundary conditions is bigger than zero, the file is read by the model. Otherwise, it is ignored. Since type-2 boundary flux is a time-dependent input, the file is structured to allow variable values with respect to time. As with all other time-dependent input files, the file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. The two node numbers of the boundary side that receives the corresponding flux is input in second and third columns of the file. In the last column, the boundary flux value is specified in cubic meters per second per meter. It must again be noted that although the flux value of a particular side might not change at some particular time level, it must still be included in each time line. Therefore, all time lines of *GWflow_bc2.txt* file must include all boundary sides regardless of a change in the flux value. In the data file, a positive flux corresponds to an outflux condition and a negative flux corresponds to an influx condition.
This file contains information regarding the type-3 boundary condition in the groundwater flow domain. A sample GWflow_bc3.txt file is shown in Figure 7.18. The file is in tab-delimited format. If the number of type-3 boundary conditions is bigger than zero, the file is read by the model. Otherwise, it is ignored. Since type-3 boundary flux is a time-dependent input, the file is structured to allow variable values with respect to time. As with all other time-dependent input files, the file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. The two node numbers of the boundary side that receives the corresponding flux is input in second and third columns of the file. The fourth and fifth columns contain the time-independent hydraulic conductivity and thickness of the sediment layer over which the type-3 boundary condition is effective. They are included for consistency purposes. The sixth column contains the time-dependent wetted perimeter of the boundary side over which the type-3 boundary condition is effective. The seventh column contains the time-independent layer bottom elevation. Finally, the last column contains the time-dependent stage value acting on the type-3 boundary side. The hydraulic conductivity and thickness of the sediment layer are given in units of meters per second and meters. The wetted perimeter, bottom elevation
and stage values are input in units of meters. It must again be noted that although the time-dependent parameters of type-3 boundary condition (i.e., wetted perimeter and stage) might not change at some particular time level, it must still be included in each time line. Therefore, all time lines of GWflow_bc3.txt file must include all boundary sides regardless of a change in the time-dependent parameter’s value.

<table>
<thead>
<tr>
<th>Time</th>
<th>Node1</th>
<th>Node2</th>
<th>K_r</th>
<th>m_r</th>
<th>w_r</th>
<th>z_r</th>
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</tr>
</thead>
<tbody>
<tr>
<td>32143.500</td>
<td>1</td>
<td>2</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>0.000001</td>
<td>0.3</td>
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<td>30</td>
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</tr>
<tr>
<td></td>
<td>4</td>
<td>5</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td>32500.500</td>
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<td>2</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
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<td>0.3</td>
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<td>30</td>
<td>31</td>
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<tr>
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<td>0.000001</td>
<td>0.3</td>
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<td>30</td>
<td>31</td>
</tr>
<tr>
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<td>3</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>5</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td>33238.500</td>
<td>1</td>
<td>2</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>3</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
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<td>4</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>5</td>
<td>0.000001</td>
<td>0.3</td>
<td>25</td>
<td>30</td>
<td>31</td>
</tr>
</tbody>
</table>

Figure 7.18. A portion of ‘GWflow_bc3.txt’ input file

- **RIVtrans_parameters.txt**

This file contains the main simulation parameters that define the contaminant transport simulation in river channels. A sample `RIVtrans_parameters.txt` file is shown in Figure 7.19. As seen from the figure, this file has a very similar format as its flow counterpart. It is a space-delimited file which is organized in two columns. The 25-character wide first column of each line includes a brief description of the data parameter that follows. The next 10 characters contain the actual data for this parameter. This format should be followed strictly for accurate data input to the model.
Figure 7.19 ‘RIVtrans_parameters.txt’ input file

The first five lines of data are exactly the same as in RIVflow_parameters.txt file. They should be exactly repeated in this file. The model is not equipped with an internal check mechanism so the user must make sure to input the same values in both files. The last two rows of data are transport model specific and are used to input the radioactive and biochemical decay constants. These are input in units of per second.

- **RIVtrans_channel_data.txt**

This file contains the channel specific data for the contaminant transport model. An example of RIVtrans_channel_data.txt file is shown in Figure 7.20. It is a space-delimited file where each channel is input in a separate row.
Following a header line, a 5-character wide column stores the channel identification number. The second column is stores a channel identification name in a 20-character wide field. The third and fourth columns are both 10-character wide fields and store the starting and ending cross-sections of the channel. The next column covers a 10-character wide space and is used to specify the Strahler order of the channel as discussed before. The next 6 columns define the boundary condition data associated with each channel. Normally, a channel could have a maximum of two boundary conditions only when the system is comprised of a single channel. For all other conditions, channels would have one or no boundary conditions depending on the relative position of the channel within the network. In the example shown in Figure 7.20., the two upstream channels (i.e., Altamaha-1 and Ohoopee) have one upstream boundary condition and the downstream channel (i.e., Altamaha-2) has one downstream boundary condition. The 5-character wide column that immediately follows the channel order is used to input whether a channel would have an upstream boundary condition or not. If an upstream boundary condition is assigned to the particular channel, then the value of this parameter is set to 1. If the channel does not have an upstream boundary condition, the value of this parameter is set to 0. If the channel has an upstream boundary condition, then the next two fields are completed, otherwise they are left empty. The first one of these two columns specifies the type of the boundary condition. The proposed model would allow the use of a specified concentration boundary condition.
at the upstream boundaries of a channel. At the downstream boundary, the model uses an advective outflux condition which does not require an input file. For the specified concentration boundary conditions, an input file is specified as shown in Figure 7.21. The file is a tab-delimited file and starts and ends the actual simulation start and end times. Following the header line, the data includes two columns separated with a tab. The first column specifies the position in time and the second column specifies the actual concentration data in milligrams per liter. The time step between two data lines is arbitrary but no two consecutive data could be closer than the minimum allowed time step. It is also important to note that a minimum of 4 timelines must be specified in a specified concentration time series data file, the first and the last of which must be the simulation starting and ending times, respectively.

![Figure 7.21. A specified concentration boundary condition file](image)

- **RIVtrans_initial_cond.txt**

This file contains the initial condition data to start the contaminant transport simulations. A portion of the sample **RIVtrans_initial_cond.txt** file is shown in Figure 7.22. Being different from its flow counterpart, this file cannot be created internally and must be supplied by the user. It is a tab-delimited file and contains two columns of data. In the first column, the cross-section identifier is input. The second column contains the initial contaminant
concentration values recorded for the cross-section. The concentration values are input in milligrams per liters.

Figure 7.22. A portion of ‘RIVtrans_initial_cond.txt’ input file

- **GWtrans_parameters.txt**

  This file contains the main simulation parameters that define the contaminant transport simulation in groundwater. A sample *GWtrans_parameters.txt* file is shown in Figure 7.23. As seen from the figure, this file has a very similar format as its flow counterpart. It is a space-delimited file which is organized in two columns. The 25-character wide first column of each line includes a brief description of the data parameter that follows. The next 10 characters contain the actual data for this parameter. This format should be followed strictly for accurate data input to the model.
The first four lines of data are exactly the same as in \textit{GWflow\_parameters.txt} file. They are repeated in this file. The model is not equipped with an internal check mechanism so the user must make sure to input the same values in both files. The next two rows of data specify the two types of boundary conditions. These are followed by data related to effective diffusion coefficient, radioactive decay coefficient and biochemical decay coefficient. The diffusion coefficient is input in square meters per second and the decay coefficients are input in units of per second.

- \textit{GWtrans\_nodes.txt}

This file contains the nodal data for groundwater transport domain. A portion of the sample \textit{GWtrans\_nodes.txt} file is shown in Figure 7.24. The file is in tab-delimited format which is organized in two columns. The first column is used to input the nodal identifier. The second column is used to input the initial contaminant concentration at the node.
GWtrans_elements.txt

This file contains the element specific data for contaminant transport in groundwater domain. A portion of the sample GWtrans_elements.txt file is shown in Figure 7.25. The file is in tab-delimited format which is organized in six columns. The first column is used to input the element identifier. The second and third columns are used to input the element dispersivity data. The fourth and fifth columns are used to input the density and porosity in the element. The sixth column is used to input portioning coefficient applicable to the element. The dispersivities are given in units of meters. The density is in kilograms per cubic meters and the portioning coefficient is in cubic meters per kilograms.
This file contains the well data for contaminant transport in groundwater domain. A sample GWtrans_wells.txt file is shown in Figure 7.26. The file is in tab-delimited format. If the number of wells data value is bigger than zero, the values inside the GWtrans_wells.txt file is read by the model. Otherwise, it is ignored. In the example shown in Figure 7.26, the domain has 5 wells located at nodes 16, 700, 1328, 3891 and 5010. Similar to well flow, the well concentration is also a time-dependent input. Therefore, the file is structured to allow variable values with respect to time. As with all time-dependent input data, the input file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. The corresponding contaminant concentrations in wells located at nodes 16, 700, 1328, 3891 and 5010 are specified for each timeline. It must be noted that when a well is a discharging well at any point in time, the concentration value specified in the input file is of no use. In such conditions, that data is ignored by the model since the concentration in the discharging well waters would be equal to the contaminant concentration in the groundwater. In this regard, the data in GWtrans_wells.txt file is used only when the well is a recharging well. For the discharging well conditions, the data is kept in the file for consistency purposes but does not have any meaningful interpretation.
This file contains the line source specific data for contaminant transport in groundwater. A portion of the sample GWtrans_lines.txt file is shown in Figure 7.27. The file is in tab-delimited format which is organized in eight columns. The user must be aware of the fact that the river network serves as a line source for the groundwater flow domain. Therefore, this file provides a link between the two flow domains. The first column is used to input the line segment identifier. The second and third columns are used to input the nodal connectivity data of the line segment. The fourth through sixth columns are used to input the vertical dispersivity and porosity of the river bottom sediments as well as the initial contaminant concentration in the line segment, respectively. The last two columns are used to input the river cross-sections that correspond to the groundwater flow nodes given in columns 2 and 3. Therefore, this file provides a mapping between the groundwater domain nodal numbering scheme and the river domain nodal numbering scheme. It is important to note that the numbering scheme should exactly follow the same order in GWflow_lines.txt file. The vertical dispersivity is input in meters. The river concentration is given in milligrams per liter.
• *GWtrans_infilt.txt*

This file contains the infiltration data for contaminant transport in groundwater domain. A portion of the sample *GWtrans_infilt.txt* file is shown in Figure 7.28. The file is in tab-delimited format. The file assigns a concentration value to all elements of the domain regardless of whether the element receives infiltration/exfiltration or not. However, the concentration value is not used when exfiltration occurs. Since infiltration concentration is a time-dependent input, the file is structured to allow variable values with respect to time. As with other time-dependent input files, the input file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. The concentration values must have units of milligrams per liter.
This file contains information regarding the type-1 boundary condition of the groundwater
transport model. A portion of the sample GWtrans_bc1.txt file is shown in Figure 7.29. The
file is in tab-delimited format. If the number of type-1 boundary conditions is bigger than
zero, the file is read by the model. Otherwise, it is ignored. Since type-1 boundary
condition is a time-dependent input, the file is structured to allow variable values with
respect to time. As with all time-dependent data, the input file must start and end with the
simulation starting and ending times. Moreover, there should at least be four time lines of
data. It must be noted that although the value of the boundary condition at a particular node
might not change at some particular time level, it must still be included in each time line.
Therefore, all time lines of GWtrans_bc1.txt file must include all boundary condition nodes
regardless of a change in the nodal hydraulic head value. In the data file, the nodal
contaminant concentration is given in milligrams per liter.
Figure 7.29. A portion of ‘GWtrans_bc1.txt’ input file

- *GWtrans_bc2.txt*

This file contains information regarding the type-2 boundary condition of the groundwater transport model. A sample *GWtrans_bc2.txt* file is shown in Figure 7.30. The file is in tab-delimited format. If the number of type-2 boundary conditions is bigger than zero, the file is read by the model. Otherwise, it is ignored. Since type-2 boundary flux is a time-dependent input, the file is structured to allow variable values with respect to time. As with all other time-dependent input files, the file must start and end with the simulation starting and ending times. Moreover, there should at least be four time lines of data. The two node numbers of the boundary side that receives the corresponding flux is input in second and third columns of the file. In the last column, the boundary flux value is specified in milligrams per meter per second. It must again be noted that although the flux value of a particular side might not change at some particular time level, it must still be included in each time line. Therefore, all time lines of *GWtrans_bc2.txt* file must include all boundary sides regardless of a change in the flux value.
7.3. Output Files

As a result of model simulations, several output files are created. These files are used to report the results of various model variables. A list of the output files created with flow and contaminant transport modules are given in Table 7.1. The file names represent the parameter that is output within the file. Only in flux output file, both the x- and y-components of Darcy velocity are printed at each node. All of the output files are tab-delimited text files that could easily be accessed with all major spreadsheet programs. All files provide a time-dependent history of the particular model parameter at each node in the discretized domain. The particular parameter output in the file is written in a matrix form such that the rows of the matrix represent the time position within the simulation and the columns represent the channel cross-section or groundwater node position within the system. Therefore, each output file provides a full spatial and temporal coverage of the particular parameter during the simulation.

<table>
<thead>
<tr>
<th>Time</th>
<th>Node1</th>
<th>Node2</th>
<th>Flux</th>
</tr>
</thead>
<tbody>
<tr>
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<td>-1.0E-5</td>
</tr>
<tr>
<td></td>
<td>2</td>
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<td>-1.0E-5</td>
</tr>
<tr>
<td></td>
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<td>4</td>
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<td>0.0E-0</td>
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<td>-2.0E-5</td>
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<td>0.0E-0</td>
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</table>

Figure 7.30. ‘GWtrans_bc2.txt’ input file
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<th>Component</th>
<th>Module</th>
<th>Output file</th>
</tr>
</thead>
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<tr>
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<td>Channel flow module</td>
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</tr>
<tr>
<td></td>
<td>Groundwater flow module</td>
<td>hydraulic_head.txt, flux.txt</td>
</tr>
<tr>
<td>Transport Model</td>
<td>Channel transport module</td>
<td>RIVconc.txt</td>
</tr>
<tr>
<td></td>
<td>Groundwater transport module</td>
<td>GWconc.txt</td>
</tr>
</tbody>
</table>

7.4. **Lower Altamaha Watershed Simulations**

The data sets that are used in simulating the flow and contaminant transport patterns in the Lower Altamaha Watershed are provided in the accompanying disk. For any potential simulations covering other time frames or different contaminant transport simulations, the user must carefully modify the input files according to the principles given in the previous sections of this appendix.
8. References


