

An Integrated Media, Integrated Processes Watershed Model – WASH123D: Part 1 – Model Descriptions and Features

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ABSTRACT

Parametric-based, lumped watershed models have been widely employed, in the past 30 years, for integrated surface and groundwater modeling to calculate surface runoff and pollution loads on various temporal and spatial scales of hydrologic regimes. Physics-based, process-level, distributed models that have the design capability to cover multimedia and multi-processes and are applicable to various scales have been practically nonexistent until recently. It has long been recognized that only such models have the potential to further the understanding of the fundamental biological, chemical, and physical factors that take place in nature hydrologic regimes; to give mechanistic predictions; and most importantly to be able to couple and interact with weather/climate models. However, there are severe limitations with these models that inhibit their use. These are, among other things, the *ad hoc* approaches of coupling between various media, the simplistic approaches of modeling water quality, and the excessive demand of computational time. This paper presents the development of an integrated media (river/stream networks, overland regime, and subsurface media), integrated processes (fluid flows and thermal, salinity, sediment, and water quality transport) watershed model to address these issues. Rigorous coupling strategies are described for interactions among overland regime, rivers/streams/canals networks, and subsurface media. Generalized paradigms of reaction-based water quality modeling are presented. Various application-dependent numerical options to simulate scalar transport are provided. A total of 32 examples were used to demonstrate the flexibility and efficiency of the model as applied to regional-level large scale and project-level small scale problems.

1. INTRODUCTION

This paper presents the development of a numerical model simulating density-dependent flow, thermal transport, salinity transport, and sediment and water quality transport in WAtERSHed Systems of One-Dimensional Stream-River Network, Two-Dimensional Overland Regime, and Three-Dimensional Subsurface Media (WASH123D). WASH123D is an integrated multimedia, multi-processes, physics-based computational model of various spatial-temporal scales.

2.3 Multimedia

WASH123D was developed to cover dendritic river/stream/canal networks and overland regime (land surface) (top plate of Fig. 1) and subsurface media including vadose and saturated (groundwater) zones (bottom plate of Fig. 1). It incorporates natural junctions and control structures such as weirs, gates, culverts, levees, and pumps in river/stream/canal networks (Fig. 2). It also includes management structures such as storage ponds, pumping stations, culverts, and levees in the overland regime. In the subsurface media, management devices such as pumping/injecting wells, drainage pipes, and drainage channels are also included. Numerous management rules of these control structures and pumping operations have been implemented.

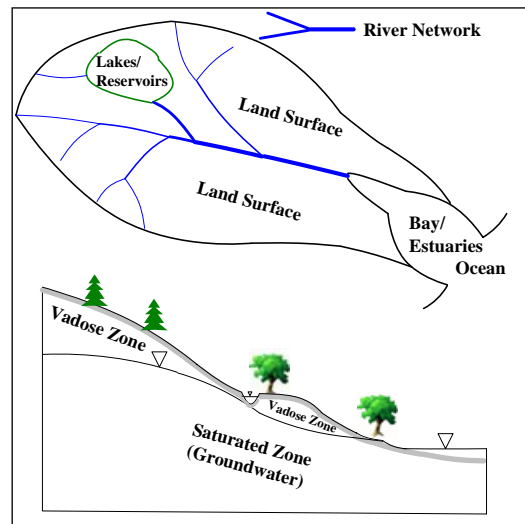


Figure 1 Multimedia in WASH123D

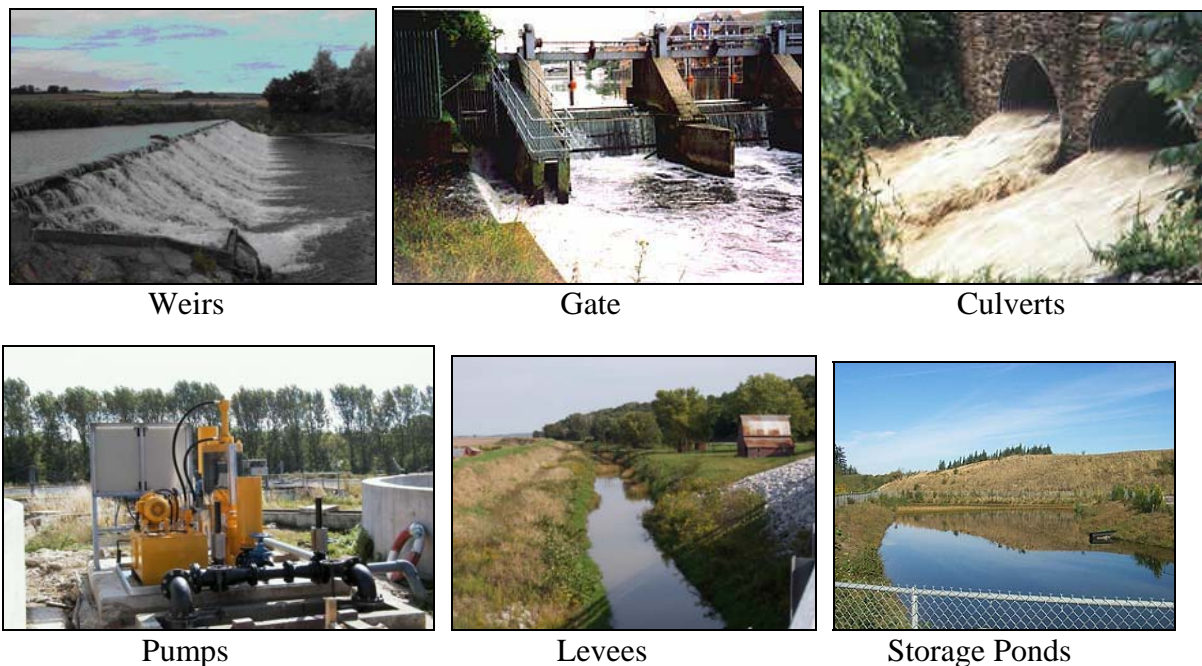


Figure 2 Various Types of Control Structures Handled in WASH123D

2.4 Multi-Processes

WASH123D is designed to deal with physics-based multi-processes occurring in watersheds. These include density dependent flow and thermal and salinity transport over the entire hydrologic cycle (Fig. 3). The processes include (1) evaporation from surface waters (rivers, lakes, reservoirs, ponds, etc) in the terrestrial environment; (2) evportranspiration from plants, grass, and forest from the land surface; (3) infiltration to vadose zone through land surface and percolations (recharges) to groundwater through water tables; (4) fluid flow

and scalar thermal/salinity transport in all media and (5) sediment transport in both overland and river networks.

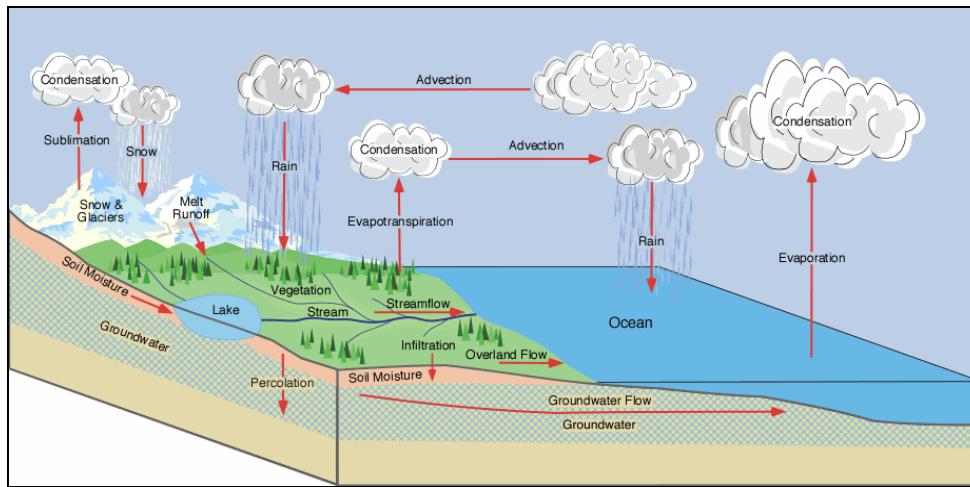


Figure 3 Hydrologic Cycle and Scalar Transports in WASH123

To enable the modeling of any number of water quality constituents a general paradigm of reaction-based approaches is taken in WASH123D. As a result of this generic approach, WASH123D can easily be employed to model biogeochemical cycles (including nitrogen, oxygen, phosphorous, and carbon cycles, etc. as shown in Figure 4 and biota kinetics (including Algae, Phytoplankton, Zooplakton, Caliform, Bacteria, Plants, etc.). In fact, once one's ability to transform biogeochemical processes into reaction networks and come up with rate equations for every reaction is achieved, one can employ WASH123D to model his/her system of reactive transport in surface runoff, surface water, and subsurface meida on watershed scales.

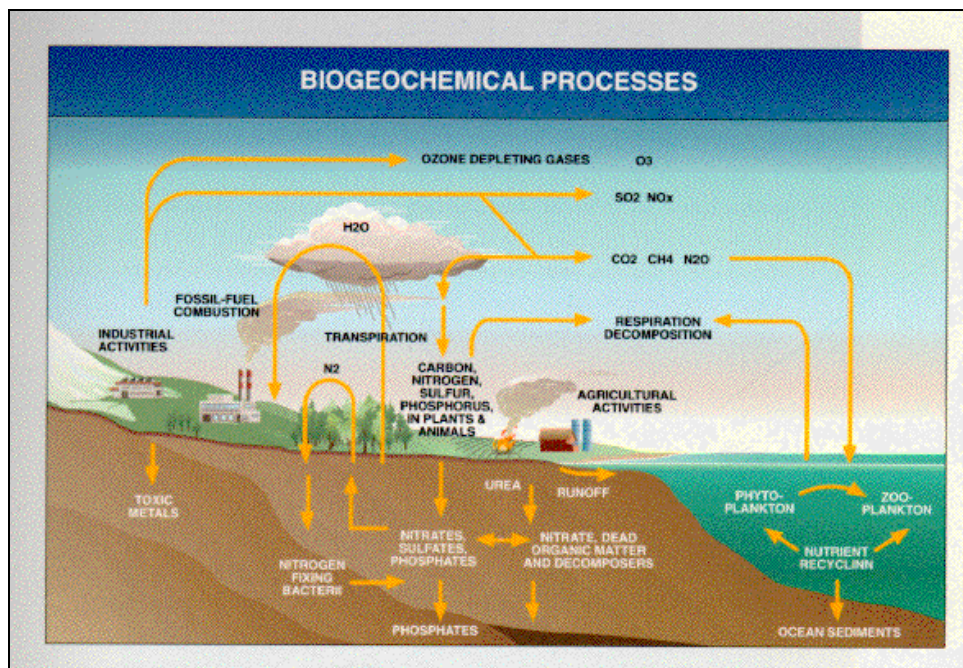


Figure 4 Biogeochemical Cycles and Reactive Transport Included in WASH123D.

2. THEORETICAL BASIS

The theoretical bases of fluid flows and transport processes built in WASH123D are based on the conservation laws of fluid, momentum, energy, and mass with associated constitute relationships between fluxes and state variables and appropriately formulated equations for source/sink terms. Various types of boundary conditions based on physics reasoning are essential to supplement governing equations. Adequate initial conditions are either obtained from measurements or with simulations of steady-state versions of governing equations.

2.1 Governing Equations

For fluid flows in river/stream/canal networks, one-dimensional St Venant Equations (Singh, 1996) modified to include the effects of density due to temperature and salinity are employed, which are in fact the cross-section area averaged Navier-Stokes equations. For surface runoff over the land surfaces, two-dimensional St Venant Equations (Singh, 1996) modified to take into account the effects of temperature- and salinity-dependent density. The two-dimensional St Venant Equations are in fact the vertically averaged Navier-Stokes equations.

The particular features in WASH123D are the inclusion of three approaches to model surface flow in a watershed system: the kinematic, diffusive, and dynamic wave models. The dynamic wave models completely describe water flow but they are very difficult to solve under some conditions (e.g., when the slope of ground surface is steep), regardless of what numerical approach is employed. On the other hand, the diffusion and/or kinematic models can handle a wide range of flow problems but are inaccurate when the inertial terms play significant roles. Thus, three options are provided in this paper: the kinematic wave model, the diffusion wave model, and the dynamic wave model to accurately compute water flow over a wide range of conditions.

The subsurface flow is described with the modified Richards equation (Li et al., 2000). The modification incorporates the effect of density due to temperature and salinity effects. The governing equation is derived based on continuity of fluid, continuity of solid mass, incompressibility of solids, and Darcy's law.

The principles of mass balance were employed to derive the modified advective-dispersive/diffusion transport equations governing the temporal-spatial distribution of salinity, water quality, suspended sediment, and bed sediment. For sediment transport, phenomenological equations for erosions and depositions are used. For biogeochemical transport, reaction rate equations can be provided based on mechanisms (pathways) or based on empirical formulations using experimental data for every slow reaction. Examples of mechanisms-based reaction rates includes forward-backward rate equations based on the collision theory, Monod-type rate equations based on the enzymatic kinetic theory (Segel, 1975), etc. Empirical rate equations include zero-order, first order, n-th order, Freundlich kinetics, etc. For every fast reaction, either the mass action equation based on the thermodynamic approach or user's defined algebraic equation can be used.

2.2 Boundary Conditions

To enable the simulation of as wide a range of problems as possible, many types of boundary conditions that can be anticipated in real-world problems are provided. These include global boundaries, internal boundaries and internal sources/sinks, and media

interfaces. On global boundaries, five types of boundary conditions can be prescribed for subsurface flow: (1) specified pressure head, (2) specified flux, (3) specified pressure gradient, (4) variable conditions in which the model will iteratively determine head or flux conditions (this type of boundary conditions is normally specified at the atmospheric boundary), and (5) radiation conditions where the flux is proportional to the difference in head between the media and surface waters such as rivers or lakes/reservoirs/ponds. For surface flow, three types of boundary conditions can be prescribed: (1) specified water depth, (2) specified flow rates, and (3) rating curves relating discharges to water depth. For scalar transport, four types of boundary conditions can be prescribed: (1) specified state variables (concentrations or temperature), (2) specified fluxes of state variables, (3) specified gradient fluxes of state variables, and (4) variable conditions in which fluxes are specified when the flow is coming into the region or the mass/energy is transported out of the region by advection when the flow is going out of the region. In addition, at the atmosphere-media interface, heat and mass budget balance must be satisfied for thermal transport.

On internal boundaries such as natural junctions and control structures of weirs, gates, culverts, levees, mass or energy balance is explicitly enforced by solving a set of flux continuity and state variable continuity (or flux) equations. For the internal sources/sinks, pumping and operation rules are simulated to ensure mass conservation.

At the interface between media, two types of connections are considered: the direct and indirect connections, as shown in Figure 5. If the change of media property near the interface can be described (resolved) by the subsurface mesh, the interface is considered as a direct connection. Otherwise, the interface is treated as an indirect connection, such as a thin layer of clay/sediment, which cannot be resolved by the subsurface mesh.

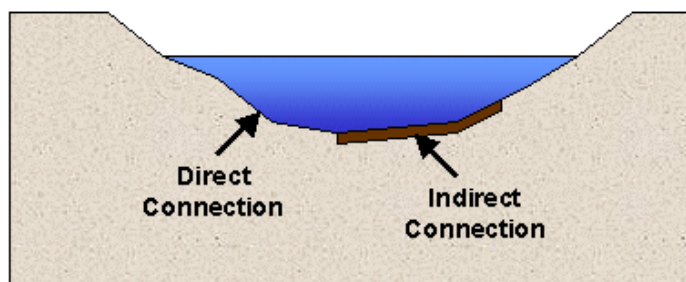


Figure 5 Two Types of Coupling between Media

3. NUMEERICAL METHODS

To provide robust and efficient numerical solutions of governing equations, many options and strategies are provided in WASH123D so a wide range of application-dependent circumstances can be simulated. For surface flow problems, the semi-Lagrangian method (backward particle tracking) was used to solve kinematic wave equations. The diffusion wave models were numerically approximated with the Galerkin finite element method or the semi-Lagrangian method. The dynamic model was first mathematically transformed into characteristic wave equations. Then it was numerically solved with the Lagrangian-Eulerian method. The subsurface flow-governing equations were discretized with the Galerkin finite element method. The dynamic wave model for surface water flows in conservative forms will be discretized with finite element methods in a future update of WASH123D.

For scalar transport equations including thermal, salinity, sediment, and reactive chemical transport, either finite element methods or hybrid Lagrangian-Eulerian methods were used to approximate the governing equations. Three strategies were employed to handle the coupling between transport and biogeochemical reactions: (1) fully implicit scheme, (2) mixed

predictor-corrector and operator-splitting methods, and (3) operator-splitting schemes. For the fully implicit scheme, one iteratively solves the transport equations and reaction equations. For the mixed predictor-corrector and operator-splitting method, the advection-dispersion transport equation is solved with the source/sink term evaluated at the previous time in the predictor step. The implicit finite difference was used to solve the system of ordinary equations governing the chemical kinetic and equilibrium reactions in the corrector step. The nonlinearity in flow and sediment transport equations is handled with the Picard method, while the nonlinear chemical system is solved using the Newton-Raphson method.

Several matrix solvers are provided to efficiently solve the system of linear algebraic equations resulting from the discretization of the governing equations and the incorporation of boundary conditions. These include direct band matrix solvers; basic point iteration solvers such as Gauss-Seidel iteration or successive over relaxation; basic line iteration solvers; preconditioned conjugate gradient methods with point iterations, incomplete Cholesky decomposition, and line iterations as preconditioners; and multigrid methods.

4. DESIGN CAPABILITY

WASH123D includes seven modules: (1) one-dimensional river/stream network module, (2) two-dimensional overland module, (3) three-dimensional subsurface module, (4) coupled 1D and 2D module, (5) coupled 2D and 3D module, (6) coupled 3D and 1D module, and (7) coupled 1D, 2D, and 3D module. Each module can be used to simulate flow alone; sediment transport alone; water quality transport alone; or flow, sediment, and water quality transport simultaneously. When both flow and transport are simulated, the flow fields are computed first. Then the transport is calculated using the computed flow fields at respective times. Temperature- and salinity-dependent flow is considered. A slightly different version of WASH123D also included 0-dimensional water, energy, and mass budget to simulate the change of stages, temperature, and concentrations of sediment and any biogeochemical species for well mixed surface water bodies such as small lakes, reservoirs, storage ponds, etc. This 0-D module has been coupled to one-dimensional canal networks and it could be coupled with two-dimensional overland regime or three-dimensional subsurface media.

5. EXAMPLE PROBLEMS

A total of 17 flow problems and 15 water quality transport problems were presented in WASH123D. These example problems can serve as templates for users to apply WASH123D to research problems or practical field-scale problems. For the 17 flow examples, the following objectives were achieved: (1) seven to demonstrate the design capability of WASH123D using seven different flow modules; (2) four to show the needs of various approaches to simulate various types of flow (critical, subcritical, and supercritical) in surface water; and (3) five to illustrate some realistic problems using WASH123D

For the 13 water quality transport problems: six examples are for one-dimensional transport, four examples for two-dimensional transport, and three examples for three-dimensional transport. These examples are used to achieve the following objectives: (1) verification of the correctness of computer implementation, (2) demonstration of the need of various numerical options and coupling strategies between transport and biogeochemical processes for application-depending circumstances, (3) illustration on how the generality of

the water quality modeling paradigm embodies the widely used water quality models as specific examples; and (4) validation of the capability of the models to simulate laboratory experiments, and indicate its potential applications to field problems.

Some of the example problems are given in a series of companion papers that are to appear in the proceeding of this conference (Huang and Yeh, 2006a, 2006b, 2006c, 2006d; Zhang and Yeh, 2006a, 2006b, 2006c). Here, because of page limit, only one example is given, which is a regional scale modeling effort of coupled surface and groundwater flow for Dade County in the South Florida wetlands.

The Dade model domain extends from four miles west of the L-67 Extension dike to the western shore of Biscayne bay and from one mile north of the Tamiami canal south to Florida bay. Vertically, it extends from the land surface to the bottom of the surficial aquifer. Some characteristics of this model are: (1) strong interaction of overland flow/groundwater flow and canal flow in south Florida and (2) complex hydraulic structure operations. The 3-D finite element mesh for subsurface media is shown in Figure 6, which consists of 37,760 global nodes and 65,429 elements. There are 7 layers in the vertical direction and levees are incorporated as part of subsurface media. Boundary conditions for subsurface flow were determined from the SFWMM 2×2 model output for the northern boundary and from structure operation records for the other sides of boundaries.

The 2-D overland flow domain consists of 4,720 nodes, and 9,347 triangular elements. Levees are included in the computation domain (Fig. 6). Boundary conditions were determined from structure operation records along the boundary. The canal network as simplified in this simulation includes: 560 canal nodes, 506 canal elements, 55 river reaches, 20 canal junctions, and 11 interior gates.

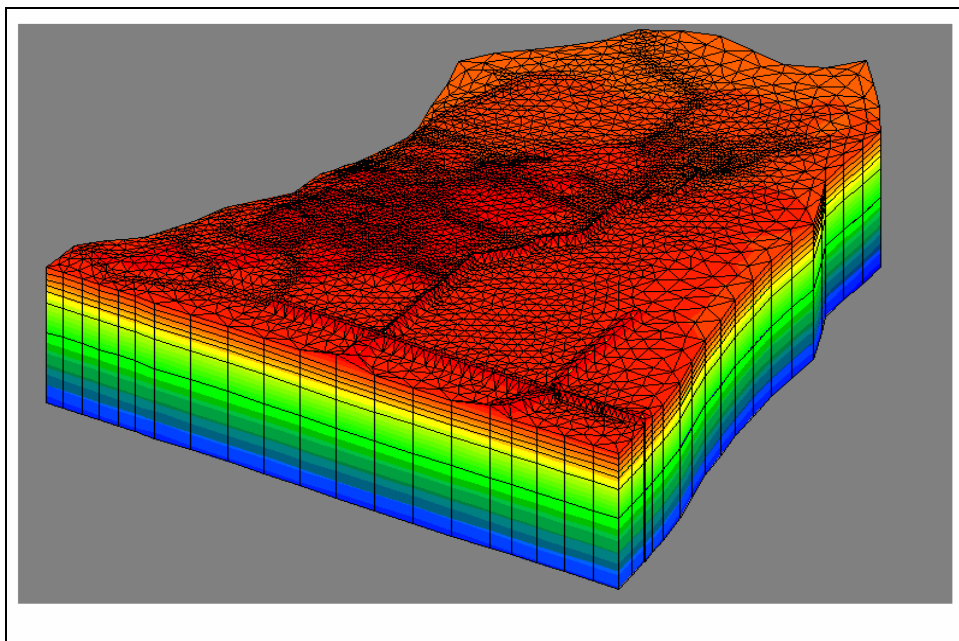


Figure 6 Three-Dimensional Subsurface Media Finite Element Mesh

The 1-D/2-D/3-D coupled flow simulation was first begun with a steady state of subsurface flow. Then the steady state condition was used as the initial condition of the transient flow simulation. Figure 7 depicts the simulations result of a model run. Since the

levee/dike are included as part of the subsurface media, it is demonstrated that the ground water flow from the northern boundary can bypass the less permeable levees via their underlying permeable media. It is also obvious that the canals recharge the ground water.

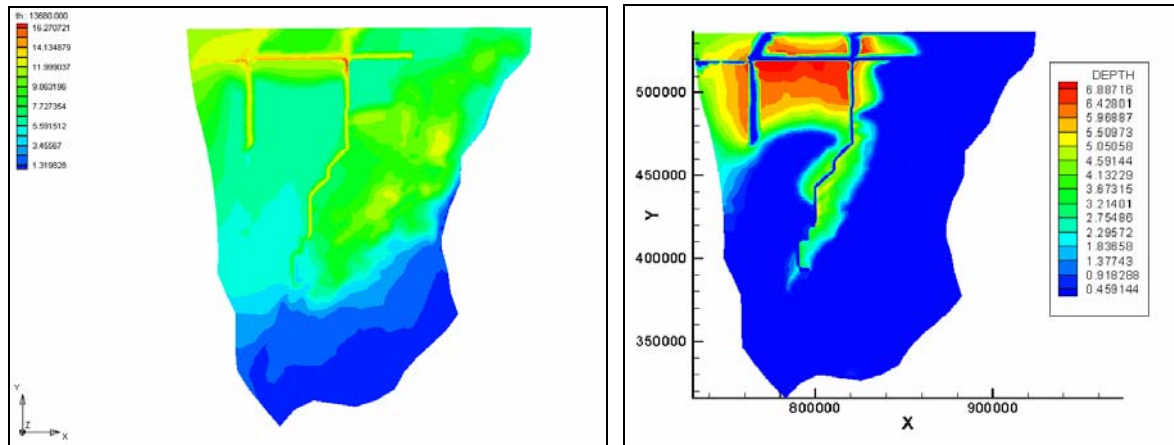


Figure 7 Left Plate - Total Head Distribution (feet) at time = 9.5 days and Right Plate - Overland Water Depth (feet) at time = 4.86 days

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