1 *INTRODUCTION*

This report is to present a numerical model designed to simulate density-dependent water flow, thermal and salinity transport, and sediment and water quality transport in watershed systems of river/stream/canal networks, overland regime, and subsurface media. WASH123D is an integrated multimedia, multi-processes, physics-based computational model of various spatial-temporal scales. The model is developed to have design capability to simulate flow and transport processes in various component systems or combinations of component systems of a watershed. It can simulate problems of various spatial and temporal scales as long as the assumptions of continuum are valid.

1.1 Multimedia

WASH123D was developed to cover dentric river/stream/canal networks and overland regime (land surface) (top plate of Fig. 1.1-1) and subsurface media including vadose and saturated (groundwater) zones (bottom plate of Fig. 1.1-1). It incorporates natural junctions and control structures such as weirs, gates, culverts, levees, and pumps in river/stream/canal networks (Fig. 1.1-2). 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.

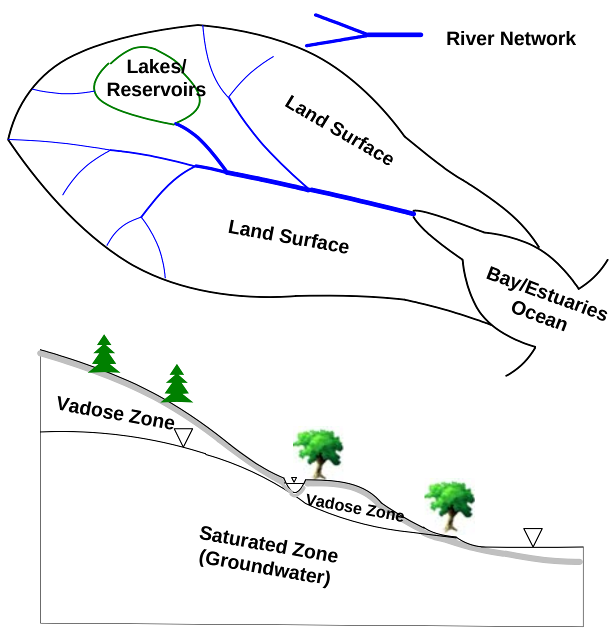

Fig. 1.1-1. Multimedia Included in WASH123D

Weirs

Gate

Culverts

Pumps

Levees

Storage Ponds

Fig. 1.1-2. Various Types of Control Structures Handled in WASH123D

1.2 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. 1.2-1). The processes include (1) evaporation from surface waters (rivers, lakes, reservoirs, ponds, etc) in the terrestrial environment; (2) evportransipiration from plants, grass, and forest from the land surface; (3) infiltration to vadose zone through land surface and recharges (percolations) to groundwater through water tables; (4) overland flow and thermal and salinity transport in surface runoff; (5) hydraulics and hydrodynamics and thermal and salinity transport in densdric river networks; and (6) subsurface flow and thermal and salinity transport in both vadose and saturated zones.

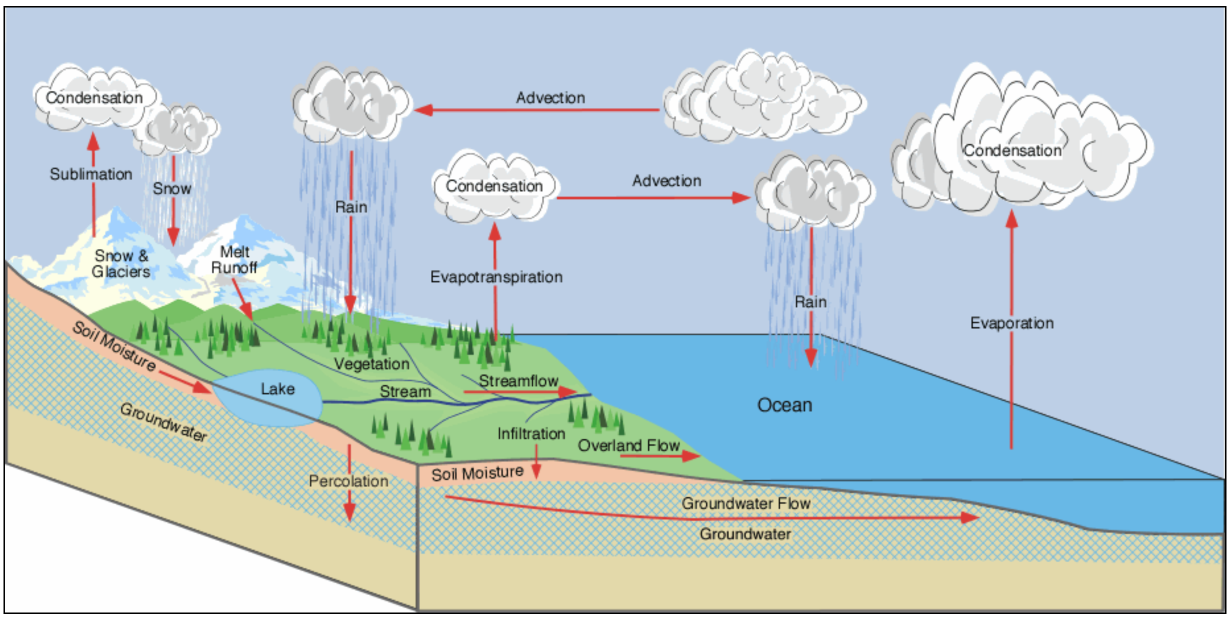

Fig. 1.2-1. Flow and Thermal and Salinity Transport Processes of Hydrologic Cycles in WASH123D

To enable the modeling of any number of water qualities including sediments, 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 bigogeochemical cycles (including nitrogen, oxygen, phosphorous, and carbon cycles, etc. as shown in Fig. 1.2-2 and biota kinetics (including Algae, Phyotoplankton, Zooplakton, Californ, 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 flows on watershed scales.

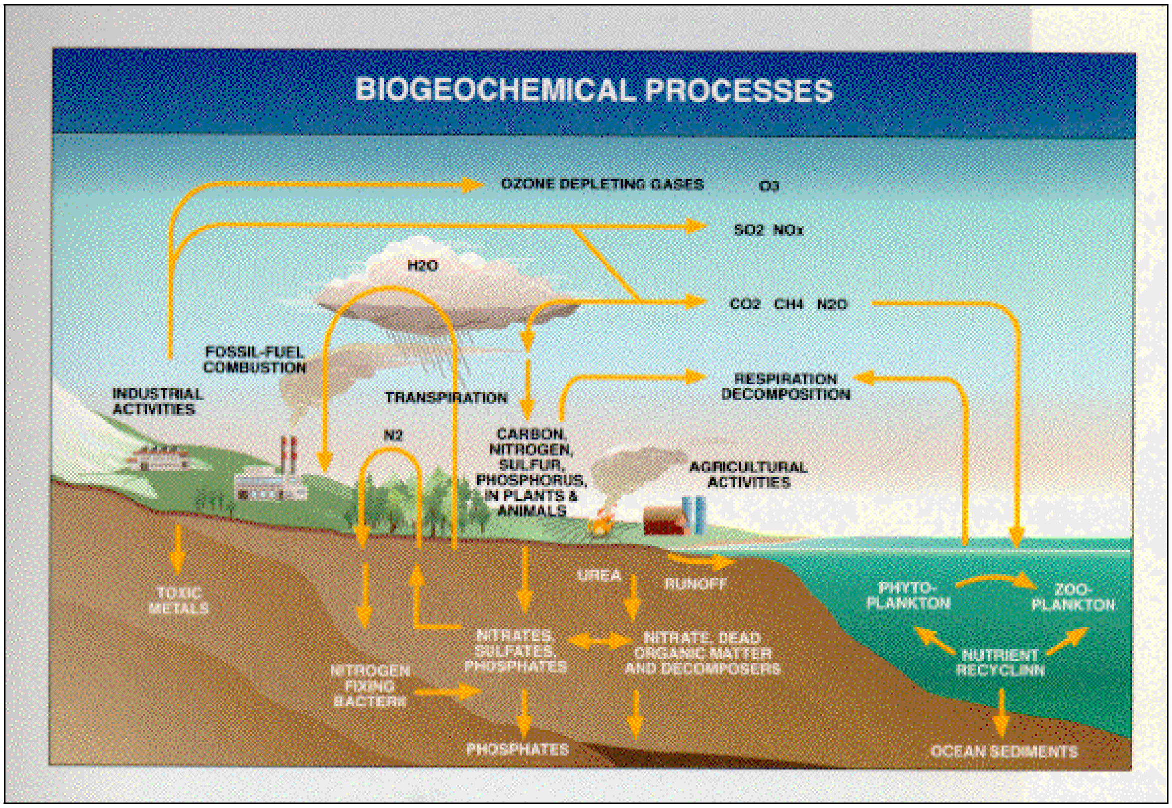

Fig. 1.2-2. Biogeochemical Cycles and Reactive Transport Included in WASH123D.

1.3 Theoretical Bases in WASH123D

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 constitution 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 the governing equations. Adequate initial conditions are either obtained from measurements or with simulations of steady-state versions of the governing equations.

1.3.1 Governing Equations

For fluid flows in river/stream/canal networks, one-dimensional St Venant Equations 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 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 report: 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. 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.

1.3.2 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 flows: (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 water flows, 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 scalor 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.

On the media interfaces, continuity of fluxes and continuity of state variables or formulations of fluxes when state variables are discontinuous are imposed.

1.3.3 Numerical Methods

To provide robust and efficient numerical solutions of the governing equations, many options and strategies are provided in WASH123D so a wide range of application-depending 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 future update of WASH123D.

For scalor 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.

1.4 Design Capability of WASH123D

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 flows alone, sediment transport alone, water quality transport alone, or flow and 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 0D module has been coupled to one-dimensional canal networks and it could be coupled with two-dimensional overland regime or three-dimensional subsurface media.

1.5 Organization of this Report

Chapter 2 provides a heuristic derivation of the governing equations and statements of boundary and initial conditions for flow in river/stream network (Section 2.1), surface runoff in the overland regime (Section 2.2), flow in the subsurface (Section 2.3) rigorous coupling of flows among various media (Section 2.4), sediment and water quality transport in river/stream network (Section 2.5), sediment and water quality transport in the overland regime (Section 2.6), water quality transport in the subsurface (Section 2.7), and coupling of transport among various media (Section 2.8).

Chapter 3 includes numerical approaches to solve governing equations for flows in the river/stream network (Section 3.1), overland (Section 3.2), and subsurface systems (Section 3.3). Numerical approximations of dynamic, diffusive, and kinematic wave models are thoroughly explored for solving flow problems in surface water. Numerical implementations of rigorously coupling fluid flow between media interfaces are addressed in Section 3.4. This chapter also describes the numerical approximation to solve both sediment and chemical transport in river/stream network (Section 3.5) and overland regimes (Section 3.6), and chemical transport in the subsurface (Section 3.7). Section 3.8 deals with detail coupling strategies in handling water quality (both sediments and biogeochemical constituents) transport problems across media interfaces. Section 3.9 presents detail computational structures of using different time-step sizes to deal with vastly different time scales of flow and transport problems in river/stream/canal networks, surface runoffs, and subsurface media.

Chapter 4 gives a total of 17 flow examples which could serve as templates for users in applying WASH123D to either research problems or real-world field applications. These examples are presented to demonstrate the design capability of WASH123D, to show the needs of various approaches to simulate flow in river networks and overland flow problems, and to illustrate some realistic problems using WASH123D.

Chapter 5 contains a total of 13 water quality transport problems: six examples for one-dimensional problems, four examples for two-dimensional problems, and three examples for three-dimensional problems. These examples are used to (1) verify the correctness of computer implementation, (2) demonstrate the need of various numerical options and coupling between transport and biogeochemical processes depending on application circumstances, (3) show the generality of the water quality modeling paradigm that embodies the widely used water quality models as specific examples, (4) validate the capability of the models to simulate laboratory experiments, and indicate its potential applications to field problems.

Summary conclusions and recommendations for further research in the development of computational models for watersheds are addressed in Chapter 6.