EXECUTIVE SUMMARY

1   INTRODUCTION

This report presents the development of a numerical model simulating density-dependent water flow, thermal transport, and salinity transport and sediment and water quality transport in watershed systems of WAterSHed Systems of 1-D Stream-River Network, 2-D Overland Regime, and 3-D Subsurface Media (WASH123D). WASH123D is an integrated multimedia, multi-processes, physics-based computational model of various spatial-temporal scales:

- **Integrated Multimedia**
  - **Dentric Streams/Rivers/Canal/Open Channel,**
  - **Overland Regime (Land Surface),**
  - **Subsurface Media (Vadose and Saturated Zones), and**
  - **Ponds, Lakes/Reservoirs (Small/Shallow)**

- **Control Structures**
  - **Weirs, Gates, Culverts, Pumps, Levees, and Storage Ponds**

- **Management: Operational Rules for Pumps and Control Structures**

- **Integrated Multi-processes**
  - **Hydrological Cycles (Evaporation, Evapotranspiration, Infiltration, and Recharges);**
  - **Fluid Flow (Surface Runoff in Land Surface, Hydraulics and Hydrodynamics in River/Stream/Canal Networks, Interflow in Vadose Zones, and Groundwater Flow in Saturated Zones);**
  - **Salinity Transport and Thermal Transport (in Surface Waters and Groundwater);**
  - **Sediment Transport (in Surface Waters);**
  - **Water Quality Transport (Any Number of Reactive Constituents);**
  - **Biogeochemical Cycles (Nitrogen, Phosphorous, Carbon, Oxygen, etc.); and**
  - **Biota Kinetics (Algae, Phyotoplankton, Zooplakton, Caliform, Bacteria, Plants, etc.)**

2   THEORETICAL BASES

Theoretical bases of WASH123D are the conservation laws of fluids, energy, mass, and biogeochemical reaction principles with physics-based constitutional relationships. The governing equations and particular features of WASH123D are given as follows:

- **Fluid Flows**
  - **1D St Venant Equations for River Networks: kinematic, diffusive, and fully dynamic (MOC) waves**
  - **2D St Venant Equations for Overland Regime: kinematic, diffusive, and fully dynamic (MOC) waves, as well as Lumped Models such as SCS**

- 3D Richard Equation for Subsurface Media (both Vadose and Saturated Zones): Saturated-unsaturated conditions

- Salinity, Thermal, and Sediment Transport
  - Modified Advection-Dispersion Equations with phenomenological approaches for erosion and deposition

- Water Quality Transport
  - Advection-Dispersion-Reaction Equations with reaction-based mechanistic approaches to water quality modeling - a general paradigm

3 TYPES OF BOUNDARY CONDITIONS

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

- Global Boundaries
  - Flows
    - For subsurface flow - specify pressure head, fluxes, pressure gradients, radiation conditions or variable boundary conditions
    - For surface flow - specify water depth, flow rate, or rating curve.
  - Salinity, Sediment, and Reactive chemical Transport
    - Specify concentration, flux, concentration gradient or variable boundary conditions.
  - Thermal Transport
    - Specify temperature, heat flux, temperature gradient or variable boundary conditions, and heat and mass budgets at the air-media interface.

- Internal Sources/sinks and Internal Boundary Conditions
  - Pumps and Operational Rules
  - Junctions - explicitly enforced mass balance
  - Control Structures - weirs, gates, culverts, levees, and storage ponds.

- Media Interfaces
  - Continuity of Fluxes Across Media Interfaces
  - Continuity of State Variables Across Media Interfaces or
  - Linkage Terms for Special Cases.

4 OPTIONAL NUMERICAL METHODS AND STRATEGIES

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. These options, strategies, and particular features are stated as follows:

- **Discretization**
  - **Flows**
    - **For subsurface flow: Use Galerkin Finite Element Methods (FEM)**
    - **For surface flow: Use Particle Tracking Methods for the kinematic wave approaches; Use Finite Element Methods or Particle Tracking Methods for the diffusive wave approaches; Use Lagrangian-Eluerian Finite Element Methods or FEM for the fully dynamic wave approaches.**
  - **Salinity, Thermal, Sediment, and Reaction-Based Water Quality Transport**
    - **Use Finite Element Methods or Particle Tracking Methods**

- **Solvers**
  - **Direct Band Matrix; Basic Point Iterations Methods; Basic Line Iterations; Preconditioned Preconditioned Conjugate Gradient Methods with Point Iterations, Incomplete Cholesky Decomposition, and Line Iterations as Preconditioners; Multigrid Methods**

- **Coupling Strategies between Transport and Reactive Chemistry**
  - **Fully Implicit Method**
  - **Mixed Prediction/Corrector (on kinetic reaction rates) and Operator-Splitting Method (on accumulation rates of immobile species)**
  - **Operator-Splitting Methods.**

In order not to introduce non-physics parameters, on the media interfaces, rigorous coupling of continuity of fluxes and continuity of state variables or formulations of fluxes when state variables are discontinuous are imposed:

- **Continuous of Fluxes**
- **Continuous of State Variables or Formulation of Fluxes**

To handle vast differences of flow and transport scales in system components of river/stream/canal networks, overland regime, and subsurface media, different time-step sizes are used.

5   DESIGN CAPABILITY OF WASH123D

The code consisted of eight modules to deal with multiple media:

(1) 1-D River/Stream Networks,
(2) 2-D Overland Regime,
(3) 3-D Subsurface Media (both Vadose and Saturated Zones);

(4) Coupled 1-D River/Stream Network and 2-D Overland Regime,
(5) Coupled 2-D Overland Regime and 3-D Subsurface,
(6) Coupled 3-D Subsurface and 1-D River Systems;

(7) Coupled 3-D Subsurface Media, 2-D Overland, and 1-D River Network; and

(8) Coupled 0-D Shallow Water Bodies and 1-D Canal Network.

For any of the above eight modules, flow only, transport only, or coupled flow and transport simulations can be carried out using WASH123D.

6   EXAMPLE PROBLEMS

A total of 17 flow problems and 15 water quality transport problems are 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 are achieved:

- **Seven to demonstrate the design capability of WASH123D using seven different flow modules;**
- **Four to show the needs of various approaches to simulate various types of flow (critical, subcritical, and supercritical) in river networks and overland regime; and**
- **Five to illustrate some realistic problems using WASH123D**

For the 13 water quality transport problems: six examples 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:

- **verify the correctness of computer implementation,**
- **demonstrate the need of various numerical options and coupling strategies between transport and biogeochemical processes for application-depending circumstances,**
- **illustrate how the generality of the water quality modeling paradigm embodies the widely used water quality models as specific examples; and**
- **validate the capability of the models to simulate laboratory experiments, and indicate its potential applications to field problems.**