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A Numerical Model Simulating Flow, Contaminant, and Sediment Transport in Watershed Systems (WASH12D)

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Prepared for U.S. Environmental Protection Agency

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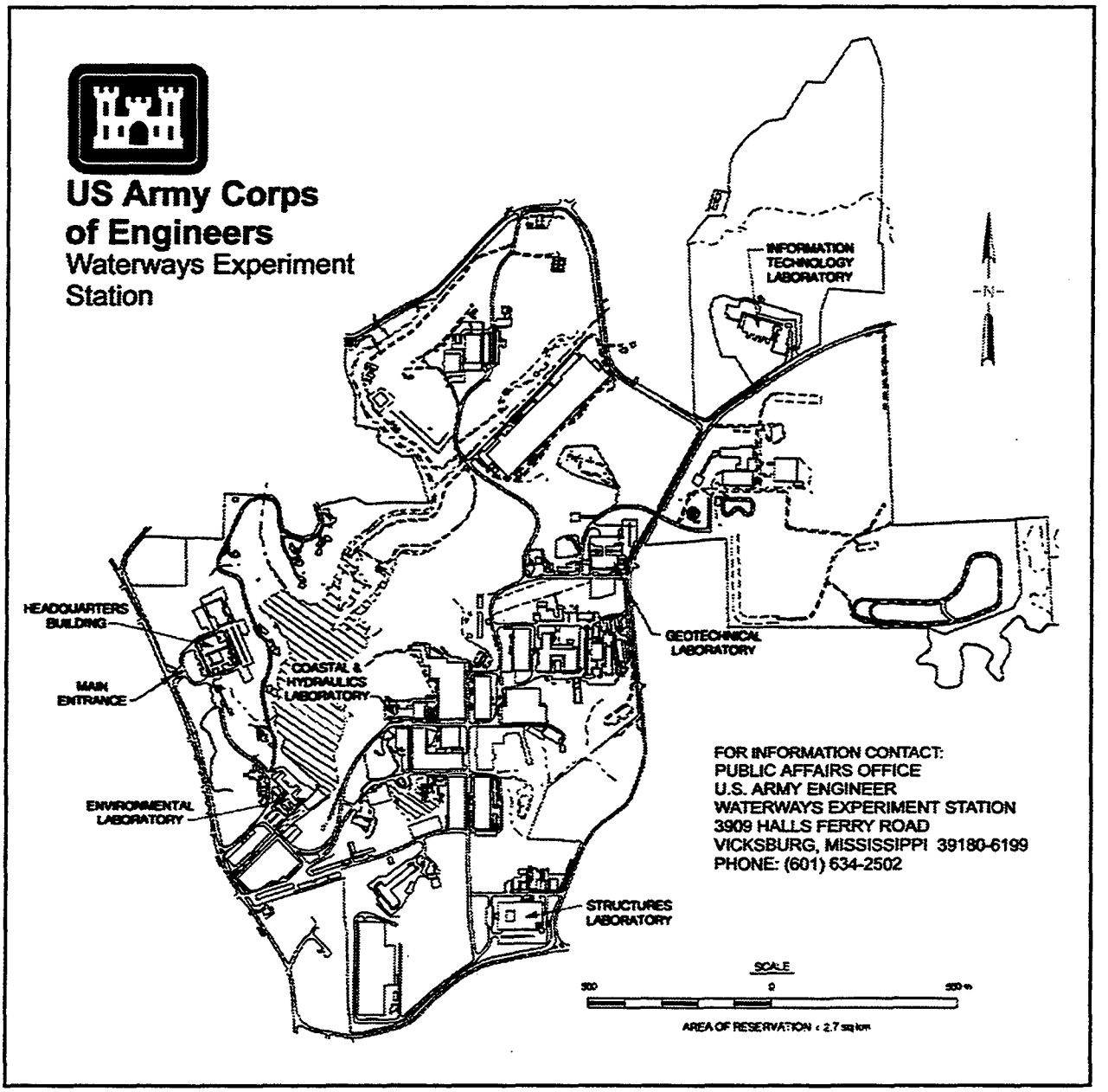

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TABLE OF CONTENTS

PREFACE	ix
SUMMARY	x
1. INTRODUCTION	Sec1-1
2. MATHEMATICAL BASIS	Sec2-1
2.1. Water flow in 1-D river/stream network	Sec2-1
2.2. Water flow in 2-D overland	Sec2-2
2.3. Contaminant and sediment transport in 1-D river/stream network	Sec2-5
2.4. Contaminant and sediment transport in 2-D overland	Sec2-9
3. NUMERICAL APPROACHES	Sec3-1
3.1. Solving the 1-D river/stream flow equations	Sec3-1
3.1.1. Method of characteristics for 1-D dynamic wave model	Sec3-1
3.1.2. The Lagrangian approach for both 1-D diffusion and 1-D kinematic wave models	Sec3-9
3.1.3. Computation of water budget at junctions	Sec3-10
3.2. Solving the 2-D overland flow equations	Sec3-11
3.2.1. Method of characteristics for 2-D dynamic wave model	Sec3-11
3.2.2. The Lagrangian approach for both 2-D diffusion and 2-D kinematic wave models	Sec3-23
3.3. Solving the 1-D river/stream transport equations	Sec3-25
3.3.1. Procedures of solving 1-D river/stream transport equations	Sec3-26
3.3.2. Determining contaminant and sediment concentrations at junctions	Sec3-31
3.3.3. Estimation of Deposition and Erosion	Sec3-33
3.4. Solving the 2-D overland transport equations	Sec3-34
4. EXAMPLES	Sec4-1
4.1. Examples of 1-D river/stream flow	Sec4-1
4.1.1. Example 1 of 1-D river/stream flow	Sec4-1
4.1.2. Example 2 of 1-D river/stream flow	Sec4-2
4.2. Examples of 2-D overland flow	Sec4-5
4.2.1. Example 1 of 2-D overland flow	Sec4-5
4.2.2. Example 2 of 2-D overland flow	Sec4-8
4.3. Example of 1-D river/stream transport	Sec4-11
4.4. Example of 2-D overland transport	Sec4-18
4.5. Example of 1-D river/stream flow and transport	Sec4-20
4.6. Example of 2-D overland flow and transport	Sec4-24
4.7. Example of 1-D/2-D flow	Sec4-32
4.8. Example of 1-D/2-D flow and transport	Sec4-37
5. SUMMARY AND CONTINUING WORKS	Sec5-1
REFERENCES	REF-1

Appendix A: DATA INPUT GUIDE AppA-1
2-D overland geometry file (.2dm files for 2-D overland simulations) AppA-1
2-D overland flow file (.2bc files for 2-D overland simulations) AppA-1
2-D overland transport files (.2tp files for 2-D overland simulations) AppA-10
1-D river/stream geometry file(.2dm files for 1-D river/stream simulations) AppA-17
1-D river/stream flow file (.2bc files for 1-D river/stream simulations) AppA-17
1-D river/stream transport file (.2tp files for 2-D overland simulations) AppA-27
1-D/2-D contaminant/sediment file (.2ch files for transport simulations) AppA-33
1-D/2-D mapping file (.map files) AppA-36

Appendix B: PROGRAM STRUCTURE AND SUBROUTINE DESCRIPTION AppB-1
Program Structure AppB-1
Subroutine Description AppB-12

Appendix C: PARAMETERS FOR RUNNING THE COMPUTER CODE AppC-1

SF 298

TABLE OF FIGURES

Figure 3.1. Tracking along characteristics in solving 1-D dynamic wave equation. Sec3-5

Figure 3.2. Tracking along characteristics in solving 2-D dynamic wave equation. Sec3-18

Figure 4.1. The bottom elevation of Example 1 of 1-D river/stream flow. Sec4-1

Figure 4.2. Water depth at various times for Example 1 of 1-D river/stream flow. Sec4-2

Figure 4.3. Discharge at various times for Example 1 of 1-D river/stream flow. Sec4-2

Figure 4.4. River/stream network for Example 2 of 1-D river/stream flow. Sec4-3

Figure 4.5. Water depth of Reach 1 at various times for Example 2 of 1-D river/stream flow. Sec4-4

Figure 4.6. Water depth of Reach 2 at various times for Example 2 of 1-D river/stream flow. Sec4-4

Figure 4.7. Water depth of Reach 3 at various times for Example 2 of 1-D river/stream flow. Sec4-4

Figure 4.8. The contour of bottom elevation for Example 1 of 2-D overland flow. Sec4-6

Figure 4.9. Discretization for Example 1 of 2-D overland flow. Sec4-6

Figure 4.10. Water depth at various times for Example 1 of 2-D overland flow. Sec4-7

Figure 4.11. Comparison of water depth between analytical solutions and numerical results for Example 2 of 2-D overland flow. Sec4-9

Figure 4.12. Comparison of velocity between analytical solutions and numerical results for Example 2 of 2-D overland flow. Sec4-10

Figure 4.13. Concentrations of (a) the first, (b) the second, and (c) the third dissolved chemicals for the example of 1-D river/stream transport. Sec4-13

Figure 4.14. Concentrations of (a) the first, (b) the second, and (c) the third suspended sediments for the example of 1-D river/stream transport. Sec4-14

Figure 4.15. Concentrations of (a) the first, (b) the second, and (c) the third bed sediments for the example of 1-D river/stream transport. Sec4-15

Figure 4.16. Concentrations of the first particulate chemical on (a) the first, (b) the second, and (c) the third suspended sediments for the example of 1-D river/stream transport. Sec4-16

Figure 4.17. Concentrations of the first particulate chemical on (a) the first, (b) the second, and (c) the third bed sediments for the example of 1-D river/stream transport. Sec4-17

Figure 4.18. Concentration contour of the first dissolved chemical at time = 260 s for the example of 2-D overland transport. Sec4-18

Figure 4.19. Concentration contour of the second dissolved chemical at time = 260 s for the example of 2-D overland transport. Sec4-19

Figure 4.20. Concentration contour of the third dissolved chemical at time = 260 s for the example of 2-D overland transport. Sec4-19

Figure 4.21. Concentration contour of the fourth dissolved chemical at time = 260 s for the example of 2-D overland transport. Sec4-19

Figure 4.22. Concentration contour of the fifth dissolved chemical at time = 260 s for the example of 2-D overland transport. Sec4-20

Figure 4.23. Concentration contour of the sixth dissolved chemical at time = 260 s for the example of 2-D overland transport. Sec4-20

Figure 4.24. Water depth at various times for the example of 1-D river/stream flow and transport. Sec4-21

Figure 4.25. Concentration of the first dissolved chemical at various times for the example of 1-D river/stream flow and transport. Sec4-22

Figure 4.26. Concentration of the second dissolved chemical at various times for the example of 1-D river/stream flow and transport. Sec4-22

Figure 4.27. Concentration of the third dissolved chemical at various times for the example of 1-D river/stream flow and transport. Sec4-22

Figure 4.28. Concentration of the fourth dissolved chemical at various times for the example of 1-D river/stream flow and transport. Sec4-23

Figure 4.29. Concentration of the fifth dissolved chemical at various times for the example of 1-D river/stream flow and transport. Sec4-23

Figure 4.30. Concentration of the sixth dissolved chemical at various times for the example of 1-D river/stream flow and transport. Sec4-23

Figure 4.31. Water depth at various times for the example of 2-D overland flow and transport. Sec4-25

Figure 4.32. Concentration of the first dissolved chemical at various times for the example of 2-D overland flow and transport. Sec4-26

Figure 4.33. Concentration of the second dissolved chemical at various times for the example of 2-D overland flow and transport. Sec4-27

Figure 4.34. Concentration of the third dissolved chemical at various times for the example of 2-D overland flow and transport. Sec4-28

Figure 4.35. Concentration of the fourth dissolved chemical at various times for the example of 2-D overland flow and transport. Sec4-29

Figure 4.36. Concentration of the fifth dissolved chemical at various times for the example of 2-D overland flow and transport. Sec4-30

Figure 4.37. Concentration of the sixth dissolved chemical at various times for the example of 2-D overland flow and transport. Sec4-31

Figure 4.38. The topography and grids for the example of 1-D/2-D flow. Sec4-33

Figure 4.39. Water depth of 1-D river/stream at various times for the example of 1-D/2-D flow. Sec4-34

Figure 4.40. Velocity of 1-D river/stream at various times for the example of 1-D/2-D flow. Sec4-35

Figure 4.41. Water depth of 2-D overland at various times for the example of 1-D/2-D flow. Sec4-36

Figure 4.42. The topography and grids for the example of 1-D/2-D flow and transport. Sec4-39

Figure 4.43. Water depth of 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-40

Figure 4.44. Water depth contour of 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-41

Figure 4.45. Concentration of the first dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-42

Figure 4.46. Concentration of the second dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-43

Figure 4.47. Concentration of the third dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-44

Figure 4.48. Concentration of the fourth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-45

Figure 4.49. Concentration of the fifth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-46

Figure 4.50. Concentration of the sixth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport. Sec4-47

Figure 4.51. Concentration of the first dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-48

Figure 4.52. Concentration of the second dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-49

Figure 4.53. Concentration of the third dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-50

Figure 4.54. Concentration of the fourth dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-51

Figure 4.55. Concentration of the fifth dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-52

Figure 4.56. Concentration of the sixth dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport. Sec4-53

Preface

The report herein was prepared for the Athens Ecosystems Research Division, Office of Research and Development, U.S. Environmental Protection Agency.

The study was conducted in the Hydraulics Laboratory (HL) of the U.S. Army Engineer Waterways Experiment Station (WES) from 1995 to 1997 under the direction of Messrs. F. A. Herrmann, Jr., Director, HL; R. A. Sager, Assistant Director, HL; and Dr. William D. Martin, Chief, Hydrosciences Division, (HD) HL.

The report was prepared by Drs. Gour-Tsyh Yeh, Hwai-Ping Cheng, and Jing-Ru Cheng, Pennsylvania State University, University Park, PA; and Dr. Hsin-Chi J. Lin, Watershed Systems Group, HD.

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At the time of publication of this report, Director of WES was Dr. Robert W. Whalin. Commander was COL Robin R. Cababa, EN.

SUMMARY

This report presents the development of a numerical model simulating water flow, contaminant transport, and sediment transport in watershed systems. A watershed system includes an overland regime, a river/stream network, and subsurface media. The model is composed of two modules: flow and transport. Three options are provided in modeling the flow module in river/stream network and overland regime: the kinematic wave approach, diffusion wave approach, and dynamic wave approach. The kinematic and diffusion wave approaches are known to be numerically robust in terms of numerical convergency and stability, i.e., they can generate convergent and stable simulations over a wide range of ground surface slopes in the entire watershed. The question is the accuracy of these simulations. The kinematic wave approach usually produces accurate solutions only over the region of steep slopes. The diffusion wave approach normally gives accurate solutions over the region of mild to steep slopes. However, neither approach has the ability to yield accurate solutions over the region of small slopes, in which the inertial forces are no longer negligible compared to the gravitational forces. The kinematic wave approach cannot even address the problems of backwater effects. On the other hand, a dynamic wave approach, having included all forces, can theoretically have the potential to generate accurate simulations over all ranges of slopes in a watershed. Unfortunately, the dynamic wave approaches are not numerically robust in terms of numerical convergency and stability. Even with the physically natural method of characteristics, not to mention the conventional finite difference and finite element methods, it is very difficult to have a convergent and stable solution over the region of steep to mild slopes. This is perhaps the reason that no fully dynamic wave models have been developed for applications to watersheds in which the ground surface slopes range from steep and mild to small. The dilemma is that: kinematic/diffusion wave approaches are numerically robust over all ranges of slopes but produce inaccurate solutions over the region of small slopes; the dynamic wave approaches can deliver accurate solutions over all ranges of slopes but are not numerically robust over the region of steep to mild slopes. Therefore, it is desirable to develop a hybrid model, in which an adaptive selection of kinematic, diffusive, or dynamic wave approaches can be made over various regions of different slopes. Such a model should deliver both numerical robustness and accuracy over all ranges of slopes in a watershed. The remaining research problem is the adaptive mechanisms: under what slopes a dynamic wave approach should be employed and under what slopes a kinematic or diffusion wave approach should be adapted automatically by the code.

In the transport module for the river/stream network and overland regime, both contaminant and sediment transport are taken into account. A sediment particle can deposit on the ground surface to become a bed sediment through deposition and resuspend back to the water body to become a suspended sediment through erosion. A contaminant species may be a dissolved chemical in water phase, an absorbed chemical on suspended sediments, or an adsorbed chemical on bed sediments. A dissolved chemical can interact with other dissolved chemicals through aqueous complexation reactions and can be adsorbed onto sediments to form

its respective particulate chemicals. Chemical kinetics based on the collision theory is used to describe the interaction among chemicals.

In solving the diffusion wave flow equations, we employed the backward method of characteristics and all the nonlinear coefficient/source/sink terms are estimated along the flow characteristics. Thus, we computed water depth by using the Lagrangian approach where fictitious particles are backward tracked. The Picard method was applied to deal with the non-linearity of the flow equations. The predictor-corrector numerical scheme was employed to solve transport equations. The Newton-Raphson method was used to solve the set of algebraic equations describing chemical kinetics among all chemical species.

A total of eight groups of example problems were given in this report to demonstrate the capability of this model. Continuing work is underway to incorporate a three-dimensional subsurface flow and chemical transport model into this watershed model. The Richards' equation and advection-dispersion reactive chemical transport equations will form the basis to simulate the subsurface flow and chemical transport module in saturated-unsaturated media. The computational module of subsurface flow and reactive chemical transport will be developed based on a model of coupled density dependent flow and chemical transport through saturated-unsaturated media.

1 INTRODUCTION

This report presents a numerical model designed to simulate water flow and contaminant and sediment transport in watershed systems. This watershed model includes a one-dimensional river/stream network flow module, a one-dimensional river/stream network transport module, a two-dimensional overland flow module, and a two-dimensional overland transport module. A three-dimensional subsurface flow and transport model is to be incorporated with the current watershed model to link surface and subsurface systems through infiltration. This watershed model can be used to simulate flows alone, sediment transport alone, reactive chemical transport alone, or flow and sediment and reactive chemical transport simultaneously. When both flow and transport are simulated, the flow fields including the velocity and water depth are computed first. Then the transport are calculated using the flow field from the flow computations at each time step. In other words, the feedback of transport on flow is not considered (e.g., no density effect is considered).

There may be three approaches to model 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 (e.g., when the slope of groundwater surface is small). 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 diffusion/kinematic wave models were numerically approximated with the Lagrangian method. The dynamic model was first mathematically transformed into characteristic wave equations. Then it was numerically solved with the Lagrangian-Eulerian method.

The principles of mass balance were employed to derive the transport equations governing the temporal-spatial distribution of chemical contaminants, suspended sediment, and bed sediment Chemical kinetics based on the collision theory was used to present the relationship between reactant and product species in all chemical reactions and volatilization. The predictor-corrector numerical scheme was used to solve the transport equations. In the predictor step, the Lagrangian-Eulerian method was employed to solve the advection-dispersion transport equation. In the corrector step, the implicit finite difference was used to solve the system of ordinary equations governing the chemical kinetic reactions. The nonlinearity in flow and sediment transport equations is handled with the Picard method, while the nonlinear chemical system is solved by using the Newton-Raphson method.

In the following, Section 2 provides a heuristic derivation of the governing equations for flow in river/stream network (Section 2.1), surface runoff in the overland regime (Section 2.2), sediment and chemical transport in river/stream network (Section 2.3), and sediment and chemical transport in the overland regime (Section 2.4). Section 3 includes numerical approaches to solve governing equations for flows in both the river/stream network and overland regime. Dynamic wave and kinematic/diffusion wave models are both given. This section also describe the numerical approximation to solve both sediment and chemical transport in river/stream network and overland

regimes. Section 4 gives 8 groups of example problems to illustrate the capability of the model. These include: (1) 1-D flow, (2) 2-D flow, (3) 1-D transport, (4) 2-D transport, (5) 1-D flow and transport, (6) 2-D flow and transport, (7) 1-D and 2-D flow, and (8) 1-D and 2-D flow and transport. A summary and continuing work are given in Section 5. A data input guide is presented in Appendix A, program structure and subroutine were described in Appendix B, and required parameters to run the model are listed in Appendix C.

2 MATHEMATICAL BASIS

In this section, governing equations, initial conditions, and boundary conditions for simulating water flow and contaminant and sediment transport in watershed systems are presented.

2.1. Water flow in 1-D river/stream

The governing equations of water flow in 1-D river/stream can be derived based on the conservation law of water mass and linear momentum [Singh, 1996], and can be written as follows.

The continuity equation:

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x} = S_S+S_R-S_I+S_1+S_2 \qquad (2.1)$$

where t is time [T]; x is the axis along the river/stream direction [L]; A is cross-sectional area of the river/stream [L^2]; Q is flow rate of the river/stream [L^3/T]; S_S is the man-induced source [L^2/T]; S_R is the source due to rainfall [L^2/T]; S_I is the sink due to infiltration [L^2/T]; S_1 and S_2 are the source terms contributed from overland flow [L^2/T].

The momentum equation:

$$\frac{\partial Q}{\partial t}+\frac{\partial uQ}{\partial x} = -gA\frac{\partial (Z_0+h)}{\partial x}+\frac{\partial F_x}{\partial x}+u^r S_R-u^i S_I+u^{Y1}S_1+u^{Y2}S_2+\frac{T^s-T^b}{\rho} \qquad (2.2)$$

where h is water depth [L]; u is river/stream velocity [L/T]; g is gravity [L/T^2]; Z_0 is bottom elevation [L]; F_x is the momentum flux due to eddy viscosity [L^4/T^2]; u^r is the velocity of rainfall along the river/stream direction [L/T]; u^i is the velocity of infiltration along the river/stream direction [L/T]; u^{Y1} and u^{Y2} are the velocity, along the river/stream direction [L/T], of water from overland to river/stream; ρ is water density [M/L^3]; T^s is surface shear stress [M/T^2]; T^b is bottom shear stress [M/T^2].

Eqs. (2.1) and (2.2) are the governing equations of a 1-D dynamic wave river/stream flow model. When the diffusion wave model is considered, however, the inertia terms along the momentum equation are assumed negligible when compared with the other terms. By further assuming negligible surface shear stress, negligible eddy viscosity, and $u^r = u^i = u^{Y1} = u^{Y2} = 0$, we approximate the river/stream velocity with the following equation (Hergarten and Neugebauer, 1995).

$$u = \frac{-1}{n}\left[\frac{R}{1+(\nabla Z_0)^2}\right]^{2/3}\frac{1}{(\nabla(Z_0+h))^{1/2}}\frac{\partial (Z_0+h)}{\partial x} \qquad (2.3)$$

where n is Manning's roughness; R is hydraulic radius [L], which is defined as $R(x,t) = R^*(x,h(x,t)) = A/P$, P is the wetted perimeter [L] and can be expressed as $P(x,t) = P^*(x,h(x,t))$.

To achieve transient simulations, either water depth or stage must be given as the initial

condition, as well as flow velocity. In addition, appropriate boundary conditions need to be specified to match the corresponding physical system. In our model, four types of boundary conditions are taken into account and are stated as follows.

Water depth- or stage-specified boundary condition: This condition is applied when either water depth or stage can be prescribed at the river/stream boundary through the simulation time of period. Such a condition can be expressed as

$$h(x_b,t) = h_b(t) \tag{2.4}$$

or

$$h(x_b,t) + Z_0(x_b) = H_b(t) \tag{2.5}$$

where x_b is the coordinate of a river/stream boundary; $h_b(t)$ is a prescribed time-dependent water depth [L]; $H_b(t)$ is a prescribed time-dependent water stage [L].

Flow rate-specified boundary condition: This condition is employed when the time-dependent incoming flow rate can be prescribed at a upstream river/stream boundary. It can be expressed as

$$Q(x_b,t) = u(x_b,t)A(x_b,t) = Q_b(t) \tag{2.6}$$

where $Q_b(t)$ is a time-dependent flow rate [L^3/T].

Water depth-dependent flow rate boundary condition: This condition is often used to describe the flow rate at a downstream river/stream boundary at which the flow rate is a function of water depth. It can be written as

$$Q(x_b,t) = u(x_b,t)A(x_b,t) = Q_b(h(x_b,t)) \tag{2.7}$$

where $Q_b(h(x_b,t))$ is a water depth-dependent flow rate [L^3/T].

Junction boundary condition: This condition is applied to a boundary of a river/stream reach when the boundary is connected to a junction. In this case, the stage of the boundary is specified as the stage of the junction. That is,

$$h(x_b,t) + Z_0(x_b) = H_{junction}(t) \tag{2.8}$$

$H_{junction}(t)$ is the water stage [L] at the junction that is computed through the computation of water budget. We will give the detail of computing $H_{junction}(t)$ in Section 3.

2.2. Water flow in 2-D overland

The governing equations of 2-D overland flow can be derived based on the conservation law of water mass and linear momentum [Wang and Connor, 1975]. The governing equations of a dynamic wave model can be written as follows.

The continuity equation:

$$\frac{\partial h}{\partial t}+\frac{\partial uh}{\partial x}+\frac{\partial vh}{\partial y} = SS+R-I \tag{2.9}$$

where h is water depth [L]; u is the x-velocity [L/T]; v is the y-velocity [L/T]; SS is the man-induced source [L/T]; R is the source due to rainfall [L/T]; I is the sink due to infiltration [L/T].

The x-momentum equation:

$$\frac{\partial uh}{\partial t}+\frac{\partial u^2h}{\partial x}+\frac{\partial uvh}{\partial y} = -gh\frac{\partial(Z_0+h)}{\partial x}+\frac{\partial F_{xx}}{\partial x}+\frac{\partial F_{yx}}{\partial y}+(u^rR-u^iI)+\frac{\tau_x^s-\tau_x^b}{\rho} \tag{2.10}$$

where Z_0 is the bottom elevation of overland [L]; u^r is the component of rainfall velocity along the x-direction [L/T]; u^i is the component of infiltration velocity along the x-direction [L/T]; F_{xx} and F_{yx} are the fluxes due to eddy viscosity along the x-direction [L^3/T^2]; τ_x^s is the component of surface shear stress along the x-direction over unit horizontal overland area [$M/L/T^2$]; τ_x^b is the component of bottom shear stress along the x-direction over unit horizontal overland area [$M/L/T^2$].

The y-momentum equation:

$$\frac{\partial vh}{\partial t}+\frac{\partial uvh}{\partial x}+\frac{\partial v^2h}{\partial y} = -gh\frac{\partial(Z_0+h)}{\partial y}+\frac{\partial F_{xy}}{\partial x}+\frac{\partial F_{yy}}{\partial y}+(v^rR-v^iI)+\frac{\tau_y^s-\tau_y^b}{\rho} \tag{2.11}$$

where v^r is the component of rainfall velocity along the y-direction [L/T]; $\dot{v}$ is the component of infiltration velocity along the y-direction [L/T]; F_{xy} and F_{yy} are the fluxes due to eddy viscosity along the y-direction [L^3/T^2]; τ_y^s is the component of surface shear stress along the y-direction over unit horizontal overland area [$M/L/T^2$]; τ_y^b is the component of bottom shear stress along the y-direction over unit horizontal overland area [$M/L/T^2$].

In Eqs. (2.10) and (2.11), it is noted that if $R > 0$, u^r and v^r are prescribed; otherwise, $u^r = u$ and $v^r = v$. Likewise, if $I < 0$, $\dot{u}$ and $\dot{v}$ are either prescribed or computed with subsurface flow models; otherwise, $u^i = u$ and $v^i = v$.

When the diffusion wave model is considered, the inertia terms in Eqs. (2.10) and (2.11) are assumed not important when compared to the others. With the further assumption that eddy viscosity is insignificant, surface shear stress is negligible, and $u^r = v^r = u^i = v^i = 0$, we approximate the velocity (u, v) as follows.

$$u = \frac{-1}{n}\left[\frac{h}{1+(\nabla Z_0)^2}\right]^{2/3}\frac{1}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial(Z_0+h)}{\partial x} \tag{2.12}$$

$$v = \frac{-1}{n}\left[\frac{h}{1+(\nabla Z_0)^2}\right]^{2/3}\frac{1}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial(Z_0+h)}{\partial y} \tag{2.13}$$

To perform transient simulations, water depth (or stage) and velocity must be given as the initial conditions. Four types of boundary conditions are implemented in our model, as described

as follows.

Water depth- or stage-specified boundary condition: This condition is applied when either water depth or stage can be prescribed at overland boundary nodes through the simulation time of period. Such a condition can be expressed as

$$h(x_b, y_b, t) = h_b(t) \tag{2.14}$$

or

$$h(x_b, y_b, t) + Z_0(x_b, y_b) = H_b(t) \tag{2.15}$$

where (x_b, y_b) is the coordinate of a overland boundary node; $h_b(t)$ is a prescribed time-dependent water depth [L]; $H_b(t)$ is a prescribed time-dependent water stage [L].

Normal flux-specified boundary condition: This condition is employed when the time-dependent incoming normal flux can be prescribed at a upstream overland boundary segment. It can be expressed as

$$-\mathbf{n}\cdot\mathbf{q}(x_b, y_b, t) = -\mathbf{n}\cdot\mathbf{V}(x_b, y_b, t)\, h(x_b, y_b, t) = q_b(t) \tag{2.16}$$

where $\mathbf{n}$ is the outward unit normal vector of the boundary segment; $\mathbf{V} = (u, v)$; $q_b(t)$ is a time-dependent normal flux [L^2/T].

Water depth-dependent normal flux boundary condition: This condition is often used to describe the outgoing normal flux at a downstream overland boundary segment at which the flux is a function of water depth. It can be written as

$$-\mathbf{n}\cdot\mathbf{q}(x_b, y_b, t) = -\mathbf{n}\cdot\mathbf{V}(x_b, y_b, t)\, h(x_b, y_b, t) = -q_b(h(x_b, y_b, t)) \tag{2.17}$$

where $q_b(h(x_b, y_b, t))$ is a water depth-dependent normal flux [L^2/T].

River/stream- or junction-related boundary condition: This condition is applied to a overland boundary segment when the boundary segment is next to a river/stream or a junction, and through the segment water may flow from overland to river/stream or from river/stream to overland, depending on the water stages at both river/stream and overland. In this occasion, the normal flux is computed based on either the water depth on the overland boundary or the difference between overland and river/stream water stages. Three cases are included in this type of boundary condition.

< Case 1 > River/stream water stage is lower than the bottom elevation of the overland boundary: In this case, water is injected to river/stream from overland. The normal flux can be expressed as

$$-\mathbf{n}\cdot\mathbf{q}(x_b, y_b, t) = -\mathbf{n}\cdot\mathbf{V}(x_b, y_b, t)\, h(x_b, y_b, t) = -q_b(h(x_b, y_b, t)) \tag{2.18}$$

where $q_b(h(x_b, y_b, t))$ is a water depth-dependent normal flux [L^2/T].

< Case 2 > River/stream water stage is higher than the bottom elevation of the overland boundary

but is lower than the water stage of the overland boundary: In this case, water is still injected to river/stream from overland. The normal flux can be expressed as

$$-\mathbf{n}\cdot\mathbf{q}(x_b,y_b,t) = -\mathbf{n}\cdot\mathbf{V}(x_b,y_b,t)\,h(x_b,y_b,t) = -q_b(\Delta H(x_b,y_b,t)) \tag{2.19}$$

$$\Delta H(x_b,y_b,t) = H(x_b,y_b,t) - H_c(x_c,t) \tag{2.20}$$

where $H(x_b,y_b,t)$ is the water stage on the overland boundary [L]; $H_c(x_c,t)$ is the water stage at the river/stream related to the overland boundary [L]; ΔH is the stage difference between river/stream and overland [L]; $q_b(\Delta H(x_b,y_b,t))$ is a stage difference-dependent normal flux [L^2/T].

< Case 3 > River/stream water stage is higher than the water stage of the overland boundary: In this case, water flows from river/stream to overland. The normal flux can be expressed as

$$-\mathbf{n}\cdot\mathbf{q}(x_b,y_b,t) = -\mathbf{n}\cdot\mathbf{V}(x_b,y_b,t)\,h(x_b,y_b,t) = q_b(\Delta H(x_b,y_b,t)) \tag{2.21}$$

$$\Delta H(x_b,y_b,t) = H_c(x_c,t) - H(x_b,y_b,t) \tag{2.22}$$

where $q_b(\Delta H(x_b,y_b,t))$ is a stage difference-dependent normal flux [L^2/T].

2.3. Contaminant and sediment transport in 1-D river/stream

The transport governing equations of both contaminants and sediments in 1-D river/stream system can be derived base on the conservation law of material mass [Yeh, 1983]. They can be written as follows.

Continuity equation for suspended sediments:

$$\frac{\partial(AS_n)}{\partial t}+\frac{\partial(QS_n)}{\partial x}-\frac{\partial}{\partial x}\left[K_x A\frac{\partial S_n}{\partial x}\right] = M_n^{s}+M_n^{os}+(R_n-D_n)P \qquad n\in[1,N_s] \tag{2.23}$$

Continuity equation for bed sediments:

$$\frac{\partial M_n}{\partial t} = D_n - R_n \qquad n\in[1,N_s] \tag{2.24}$$

Continuity equation for dissolved chemicals:

$$\frac{\partial(AC_i^{w})}{\partial t}+\frac{\partial(QC_i^{w})}{\partial x}-\frac{\partial}{\partial x}\left[K_x A\frac{\partial C_i^{w}}{\partial x}\right]$$

$$= M_i^{cw}-\lambda_i^{w}AC_i^{w}+Ak_i^{ab}\left(p_i-\frac{k_i^{af}}{k_i^{ab}}C_i^{w}\right)+\sum_{n=1}^{N_s}k_{ni}^{sb}S_nA\left(C_{ni}^{s}-\frac{k_{ni}^{sf}}{k_{ni}^{sb}}C_i^{w}\right)+M_i^{crw}-M_i^{ciw}+M_i^{cow} \tag{2.25}$$

$$+\sum_{n=1}^{N_s}k_{ni}^{bb}M_nP\left(C_{ni}^{b}-\frac{k_{ni}^{bf}}{k_{ni}^{bb}}C_i^{w}\right)+\sum_{m=1}^{N_{rx}}(a_{mj}-b_{mj})k_m^{rb}A\left[\prod_{j=1}^{N_c}(C_j^{w})^{b_{mj}}-\frac{k_m^{rf}}{k_m^{rb}}\prod_{j=1}^{N_c}(C_j^{w})^{a_{mj}}\right] \qquad i\in[1,N_c]$$

Continuity equation for particulate chemicals on suspended sediments:

$$\frac{\partial(AS_nC_{ni}^s)}{\partial t}+\frac{\partial(QS_nC_{ni}^s)}{\partial x}-\frac{\partial}{\partial x}\left[K_xA\frac{\partial(S_nC_{ni}^s)}{\partial x}\right]$$

$$=M_{ni}^{cs}-\lambda_{ni}^sAS_nC_{ni}^s-k_{ni}^{sb}S_nA\left(C_{ni}^s-\frac{k_{ni}^{sf}}{k_{ni}^{sb}}C_i^w\right)+R_nBC_{ni}^b-D_nBC_{ni}^s+M_{ni}^{cos} \qquad (2.26)$$

$$n\in[1,N_s],\ i\in[1,N_c]$$

Continuity equation for particulate chemicals on bed sediments:

$$\frac{\partial(M_nC_{ni}^b)}{\partial t}=(D_nC_{ni}^s-R_nC_{ni}^b)-\lambda_{ni}^bM_nC_{ni}^b-k_{ni}^{bb}M_n\left[C_{ni}^b-\frac{k_{ni}^{bf}}{k_{ni}^{bb}}C_i^w\right] \qquad n\in[1,N_s],i\in[1,N_c] \quad (2.27)$$

where

A = River/stream cross-sectional area [L^2];

a_{mj} = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a reactant chemical;

B = Top river/stream width [L];

b_{mj} = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a product chemical;

C_i^w = Cross-sectionally-averaged concentration of the I-th dissolved chemical [M/L^3];

C_i^{rw} = Concentration of the I-th dissolved chemical in rainfall [M/L^3];

C_i^{sw} = Concentration of the I-th dissolved chemical in the subsurface [M/L^3];

C_{ni}^b = Cross-sectionally-averaged particulate chemical concentration on bed sediment of the n-th fraction size [M/M];

C_{ni}^s = Cross-sectionally-averaged particulate chemical concentration on suspended sediment of the n-th fraction size [M/M];

D_n = Deposition rate of the n-th size fraction sediment [$M/L^2/T$];

I = Infiltration from river/stream to subsurface [L^2/T];

K_x = Longitudinal dispersion coefficient [L^2/T];

k_i^{ab} =Backward volatilization rate constant associated with the I-th dissolved chemical in the atmosphere [$M/atm/L^3/T$];

k_i^{af} = Forward volatilization rate constant associated with the I-th dissolved chemical in the atmosphere [1/T];

k_{ni}^{sb} = Backward adsorption rate constant associated with the I-th particulate chemical on suspended sediment of the n-th fraction size [1/T];

k_{ni}^{sf} = Forward adsorption rate constant associated with the I-th particulate chemical on suspended sediment of the n-th fraction size [$L^3/M/T$];

k_m^{rb} = Backward rate constant of the m-th aqueous complexation reaction [reaction-dependent];

k_m^{rf} = Forward rate constant of the m-th aqueous complexation reaction [reaction-dependent];

k_{ni}^{bb} = Backward adsorption rate constant associated with the I-th particulate chemical on

suspended sediment of the n-th fraction size [1/T];

k_{ni}^{bf} = Forward adsorption rate constant associated with the I-th particulate chemical on bed sediment of the n-th fraction size [$L^3/M/T$];

M_n = Sediment mass per unit bed area of the n-th size fraction [M/L^2];

M_n^s =Source of the n-th size fraction sediment [M/L/T];

M_n^{os} = Source of the n-th size fraction sediment from overland [M/L/T]; It is equal to $R_1S_n^{os1}+R_2S_n^{os2}$, where S_n^{os1} and S_n^{os2} are the associated suspended sediment concentration of the n-th size fraction from overland.

M_{ni}^{cs} = Source of the I-th particulate chemical on suspended sediment of the n-th fraction size [M/L/T];

M_{ni}^{cos} = Source of the I-th particulate chemical on suspended sediment of the n-th fraction size from overland [M/L/T]; It is equal to $R_1S_n^{os1}C_{ni}^{os1}+R_2S_n^{os2}C_{ni}^{os2}$, where C_{ni}^{os1} and C_{ni}^{os2} are the associated I-th particulate chemical concentration on suspended sediment of the n-th size fraction from overland.

M_i^{cw} = Source of the I-th dissolved chemical [M/L/T];

M_i^{crw} =Rainfall source of the I-th dissolved chemical [M/L/T]; It is equal to RC_i^{rw} if R is positive. Otherwise, it is zero.

M_i^{ciw} =Infiltration sink of the I-th dissolved chemical [M/L/T]. It is equatl to IC_i^w if I is positive. Otherwise, it is IC_i^{sw} representing a source from the subsurface

M_i^{cow} = Source of the I-th dissolved chemical from overland [M/L/T]; it is equal to $R\,C_i^{ow1}+R\,C_i^{ow2}$, where C_i^{ow1} and C_i^{ow2} are the associated I-th dissolved chemical concentrations from overland.

N_c = Number of dissolved chemicals;

N_s = Number of sizes of sediments;

P = Wetted perimeter [L];

p_i = Partial pressure of the I-th dissolved chemical in the atmosphere [atm];

Q = River/stream flow rate [L^3/T];

R = Rainfall to river/stream [L^2/T];

R_n = Erosion rate of the n-th size fraction sediment [$M/L^2/T$];

R_1, R_2 = Surface runoff from overland to river/stream [L^2/T]; the subscripts 1 and 2 are used to differentiate the flows through the two river/stream-overland interfaces because they usually are not the same in practice.

S_n = Cross-sectionally-averaged sediment concentration of the n-th fraction size [M/L^3];

t = Time [T];

x = River/stream coordinate [L];

λ_{ni}^b = Combined first order degradation rate constant of the I-th particulate chemical on bed sediment of the n-th fraction size [1/T];

λ_{ni}^s = Combined first order degradation rate constant of the I-th particulate chemical on suspended sediment of the n-th fraction size [1/T];

λ_i^w = Combined first order degradation rate constant of the I-th dissolved chemical [1/T];

In obtaining Eqs. (2.25) through (2.27), the following reactions are considered.

(1) Aqueous complexation reactions: k_m^{rb} and k_m^{rf} as backward and forward reaction rate constants.

$$\sum_{j=1}^{N_c} a_{mj}\overline{C_j^w} \rightleftharpoons \sum_{j=1}^{N_c} b_{mj}\overline{C_j^w} \qquad m\in[1,N_{rx}] \tag{2.28}$$

$$R = k_m^{rf}\prod_{j=1}^{N_c}(C_j^w)^{a_{mj}} - k_m^{rb}\prod_{j=1}^{N_c}(C_j^w)^{b_{mj}} \tag{2.29}$$

where R is defined as the reaction rate of the aqueous complexation reaction.

(2) Adsorption/desorption between the dissolved phase and suspended sediment: k_{ni}^{sb} and k_{ni}^{sf} as backward and forward reaction rate constants.

$$\overline{C_i^w}+\overline{S_n} \rightleftharpoons \overline{C_{ni}^s}+\overline{S_n} \qquad i\in[1,N_c],n\in[1,N_s] \tag{2.30}$$

$$R = k_{ni}^{sf}S_n C_i^w - k_{ni}^{sb}S_n C_{ni}^s \tag{2.31}$$

where R is defined as the reaction rate of the adsorption reaction.

(3) Adsorption/desorption between the dissolved phase and bed sediment: k_{ni}^{bb} and k_{ni}^{bf} as backward and forward reaction rate constants.

$$\overline{C_i^w}+\overline{M_n} \rightleftharpoons \overline{C_{ni}^b}+\overline{M_n} \qquad i\in[1,N_c],n\in[1,N_s] \tag{2.32}$$

$$R = k_{ni}^{bf}M_n PC_i^w - k_{ni}^{bb}M_n PC_{ni}^b \tag{2.33}$$

where R is defined as the reaction rate of the adsorption reaction.

(4) Volatilization between the dissolved phase and atmosphere: k_i^{ab} and k_i^{af} as backward and forward reaction rate constants.

$$\overline{C_i^w} \rightleftharpoons \overline{p_i} \qquad i\in[1,N_c] \tag{2.34}$$

$$R = k_i^{af}C_i^w - k_i^{ab}p_i \tag{2.35}$$

where R is defined as the reaction rate of the volatilization reaction. In Eqs. (2.28), (2.30), (2.32), and (2.34), the over-line is used to present the formula, rather than the concentration, of a chemical or a sediment.

The concentrations of all contaminant species and sediments must be given initially for transient simulations. In our model, both bed sediments and particulate chemicals sorbed on the bed sediments are considered to be immobile, as described by Eqs. (2.24) and (2.27). Therefore, boundary conditions are needed for suspended sediments, dissolved chemicals, and particulate chemicals on suspended sediments. Four types of boundary conditions are taken into account as stated as follows.

Dirichlet boundary condition: This conditions is applied when concentration is given at the boundary. That is,

$$C(x_b,t) = C_b(t) \tag{2.36}$$

where C can be the S_n, C_i^w, or $S_nC_{ni}^s$; $C_b(t)$ is a time-dependent concentration [M/L^3].

Variable boundary condition: This boundary condition is employed when the flow direction would change with time during simulations. Two cases are considered, regarding to the flow direction on the boundary.

< Case 1 > Flow is coming in from outside:

$$\left[QC(x_b,t) - AK_x\frac{\partial C(x_b,t)}{\partial x}\right] = QC_b(t) \tag{2.37}$$

< Case 2 > Flow is going out from inside:

$$-AK_x\frac{\partial C(x_b,t)}{\partial x} = 0 \qquad \text{on } B_V \tag{2.38}$$

where $C_b(t)$ is a time-dependent concentration [M/L^3] which is associated with the incoming flow.

Cauchy boundary condition: This boundary condition is employed when the total material flow rate is given at the river/stream boundary. Usually, this boundary is a upstream boundary node. The conditions can be expressed as

$$n\left[QC(x_b,t) - AK_x\frac{\partial C(x_b,t)}{\partial x}\right] = Q_b^c(t) \tag{2.39}$$

where $Q_b^c(t)$ is material flow rate [M/T]; n = 1 if the boundary is a upstream boundary node, or n = -1 if it is a downstream boundary node.

Neumann boundary condition: This boundary condition is used when the diffusive material flow rate is known at the river/stream boundary node. It can be written as

$$-nAK_x\frac{\partial C(x_b,t)}{\partial x} = Q_b^c(t) \tag{2.40}$$

where $Q_b^c(t)$ is material flow rate [M/T].

2.4. Contaminant and sediment transport in 2-D overland

The equations governing contaminant and sediment transport in 2-D overland can be derived according to the conservation law of material mass. They can be written as follows.

Continuity equation for suspended sediments:

$$\frac{\partial(hS_n)}{\partial t}+\nabla\cdot(\mathbf{q}S_n) = \nabla\cdot\left[h\mathbf{K}\cdot\nabla S_n\right]+M_n^s+(R_n-D_n) \qquad n\in[1,N_s] \tag{2.41}$$

Continuity equation for bed sediments:

$$\frac{\partial M_n}{\partial t} = D_n-R_n \qquad n\in[1,N_s] \tag{2.42}$$

Continuity equation for dissolved chemicals:

$$\begin{aligned}&\frac{\partial(hC_i^w)}{\partial t}+\nabla\cdot(\mathbf{q}C_i^w)\\ &= \nabla\cdot\left[h\mathbf{K}\cdot\nabla C_i^w\right]+M_i^{cw}-\lambda_i^w hC_i^w+hk_i^{ab}\left(p_i-\frac{k_i^{af}}{k_i^{ab}}C_i^w\right)+\sum_{n=1}^{N_s}k_{ni}^{sb}S_n h\left(C_{ni}^s-\frac{k_{ni}^{sf}}{k_{ni}^{sb}}C_i^w\right)\\ &+\sum_{n=1}^{N_s}k_{ni}^{bb}M_n\left(C_{ni}^b-\frac{k_{ni}^{bf}}{k_{ni}^{bb}}C_i^w\right)+\sum_{m=1}^{N_{rx}}(a_{mj}-b_{mj})k_m^{rb}h\left[\prod_{j=1}^{N_c}(C_j^w)^{b_{mj}}-\frac{k_m^{rf}}{k_m^{rb}}\prod_{j=1}^{N_c}(C_j^w)^{a_{mj}}\right]\\ &+M_i^{crw}-M_i^{ciw} \qquad i\in[1,N_c]\end{aligned} \tag{2.43}$$

Continuity equation for particulate chemical on suspended sediments:

$$\begin{aligned}&\frac{\partial(hS_nC_{ni}^s)}{\partial t}+\nabla\cdot(\mathbf{q}S_nC_{ni}^s)\\ &= \nabla\cdot\left[h\mathbf{K}\cdot\nabla(S_nC_{ni}^s)\right]+M_{ni}^{cs}-\lambda_{ni}^s hS_nC_{ni}^s-k_{ni}^{sb}S_nh\left(C_{ni}^s-\frac{k_{ni}^{sf}}{k_{ni}^{sb}}C_i^w\right)\\ &+R_nC_{ni}^b-D_nC_{ni}^s \qquad n\in[1,N_s],\ i\in[1,N_c]\end{aligned} \tag{2.44}$$

Continuity equation for particulate chemical on bed sediments:

$$\frac{\partial(M_nC_{ni}^b)}{\partial t} = (D_nC_{ni}^s-R_nC_{ni}^b)-\lambda_{ni}^bM_nC_{ni}^b-k_{ni}^{bb}M_n\left[C_{ni}^b-\frac{k_{ni}^{bf}}{k_{ni}^{bb}}C_i^w\right] \qquad n\in[1,N_s],i\in[1,N_c] \tag{2.45}$$

where

h = Water depth [L];

a_{mj} = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a reactant chemical;

b_{mj} = Stoichiometric coefficient of the j-th dissolved chemical in the m-th aqueous complexation reaction when this dissolved chemical appears as a product chemical;

C_i^w = Depth-averaged concentration of the I-th dissolved chemical [M/L^3];

C_i^{rw} = Concentration of the I-th dissolved chemical in rainfall [M/L^3];

C_i^{sw} = Concentration of the I-th dissolved chemical in the subsurface [M/L^3];

C_{ni}^{b} = Depth-averaged particulate chemical concentration on bed sediment of the n-th fraction size [M/M];

C_{ni}^{s} = Depth-averaged particulate chemical concentration on suspended sediment of the n-th fraction size [M/M];

D_n = Deposition rate of the n-th size fraction sediment [$M/L^2/T$];

I = Infiltration from overland to subsurface [L/T];

K = Dispersion coefficient tensor [L^2/T];

k_i^{ab} = Backward volatilization rate constant associated with the I-th dissolved chemical in the atmosphere [$M/atm/L^3/T$];

k_i^{af} = Forward volatilization rate constant associated with the I-th dissolved chemical in the atmosphere [1/T];

k_{ni}^{sb} = Backward adsorption rate constant associated with the I-th particulate chemical on suspended sediment of the n-th fraction size [1/T];

k_{ni}^{sf} = Forward adsorption rate constant associated with the I-th particulate chemical on suspended sediment of the n-th fraction size [$L^3/M/T$];

k_m^{rb} = Backward rate constant of the m-th aqueous complexation reaction [reaction-dependent];

k_m^{rf} = Forward rate constant of the m-th aqueous complexation reaction [reaction-dependent];

k_{ni}^{bb} = Backward adsorption rate constant associated with the I-th particulate chemical on suspended sediment of the n-th fraction size [1/T];

k_{ni}^{bf} = Forward adsorption rate constant associated with the I-th particulate chemical on bed sediment of the n-th fraction size [$L^3/M/T$];

M_n = Sediment mass per unit bed area of the n-th size fraction [M/L^2];

M_n^s = Source of the n-th size fraction sediment [$M/L^2/T$];

M_{ni}^{cs} = Source of the I-th particulate chemical on suspended sediment of the n-th fraction size [$M/L^2/T$];

M_i^{cw} = Source of the I-th dissolved chemical [$M/L^2/T$];

M_i^{crw} = Rainfall source of the I-th dissolved chemical [$M/L^2/T$]. It is equal to rC_i^{rw} if r is positive. Otherwise, it is zero.

M_i^{ciw} =Infiltration sink of the I-th dissolved chemical [$M/L^2/T$]. It is equal to iC_i^{w} if I is positive. Otherwise, it is iC_i^{sw} representing a source from the subsurface.

N_c = Number of dissolved chemicals;

N_s = Number of sizes of sediments;

p_i = Gaseous pressure in the atmosphere associated with the I-th dissolved chemical [atm];

q = Flux of overland flow [L^2/T];

R = Rainfall to overland [L/T];

R_n = Erosion rate of the n-th size fraction sediment [$M/L^2/T$];

S_n = Depth-averaged sediment concentration of the n-th fraction size [M/L^3];

SS = External source/sink [L/t];

t = Time [T];

(x,y) = Horizontal coordinates [L];

λ_{ni}^{b} = Combined first order degradation rate constant of the I-th particulate chemical on bed sediment of the n-th fraction size [1/T];

λ_{ni}^{s} = Combined first order degradation rate constant of the I-th particulate chemical on

suspended sediment of the n-th fraction size [1/T];

λ_i^w =Combined first order degradation rate constant of the I-th dissolved chemical [1/T];

In obtaining the above equations, the reactions described with Eqs. (2.28) through (2.35) are considered. To achieve transient simulations, the concentrations of contaminants and sediments must be provided initially. Four types of boundary conditions can be used for mobile materials, i.e., suspended sediments, dissolved chemicals, and particulate chemicals on suspended sediments. These four boundary conditions are

Dirichlet boundary condition: This conditions is applied when concentration is given at the boundary. That is,

$$C(x_b,y_b,t) = C_b(t) \tag{2.46}$$

where C can be the S_n, C_i^w, or $S_nC_{ni}^s$; $C_b(t)$ is a time-dependent concentration [M/L^3].

Variable boundary condition: This boundary condition is employed when the flow direction would change with time during simulations. Two cases are considered, regarding to the flow direction on the overland boundary segment.

< Case 1 > Flow is coming in from outside:

$$-\mathbf{n}\cdot\left[\mathbf{q}C(x_b,y_b,t) - h\mathbf{K}\cdot\nabla C(x_b,y_b,t)\right] = -\mathbf{n}\cdot\mathbf{q}C_b(t) \tag{2.47}$$

< Case 2 > Flow is going out from inside:

$$\mathbf{n}\cdot\left(-h\mathbf{K}\cdot\nabla C(x_b,y_b,t)\right) = 0 \tag{2.48}$$

where $\mathbf{n}$ is the outward unit normal vector of the boundary segment; $C_b(t)$ is a time-dependent concentration [M/L^3], which is associated with the incoming flow.

Cauchy boundary condition: This condition is applied when the total incoming material flux is prescribed as a function of time on an overland boundary segment. It can be written as

$$-\mathbf{n}\cdot\left[qC(x_b,y_b,t) - h\mathbf{K}\cdot\nabla C(x_b,y_b,t)\right] = q_b^c(t) \tag{2.49}$$

where $q_b^c(t)$ is a time-dependent Cauchy flux [M/T/L]

Neumann boundary condition: This conditions is employed when the incoming diffusive material flux can be prescribed on a boundary segment. It is written as

$$-\mathbf{n}\cdot\left(-h\mathbf{K}\cdot\nabla C(x_b,y_b,t)\right) = q_b^c(t) \tag{2.50}$$

where $q_b^c(t)$ is a time-dependent Neumann flux [M/T/L].

3 NUMERICAL APPROACHES

In this section, the numerical approaches employed to solve the governing equations of flow and transport given in the previous section are presented.

3.1. Solving the 1-D river/stream flow equations

As mentioned earlier in this report, we desire to implement a hybrid model to accurately simulation surface water flow under a wide range of physical conditions though it is still under investigation and further study is required. In our investigation to date, we would apply the method of characteristics to solve the dynamical wave model and would use the Lagrangian approach to solve both the diffusion wave and the kinematic wave models in the hybrid model that is composed of the aforementioned three wave models. In this and the next subsections, we will present the numerical approaches used in the method of characteristics and the Lagragian approach for solving the 1-D river/stream flow and 2-D overland flow equations, respectively. In either approach, the Picard method is employed to deal with the nonlinearity.

3.1.1. Method of characteristics for 1-D dynamic wave model

Recall Eqs. (2.1) and (2.2),

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x} = S_S+S_R-S_I+S_1+S_2 \tag{3.1}$$

$$\frac{\partial Q}{\partial t}+\frac{\partial uQ}{\partial x} = -gA\frac{\partial(Z_0+h)}{\partial x}+\frac{\partial F_x}{\partial x}+u^{r}S_R-u^{i}S_I+u^{Y1}S_1+u^{Y2}S_2+\frac{T^{s}-T^{b}}{\rho} \tag{3.2}$$

We also have

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x} = B_t\frac{\partial h}{\partial t}+\frac{\partial(uhB_a)}{\partial x} \tag{3.3}$$

$$\frac{\partial B_a}{\partial x} = \frac{\partial B_a^{*}}{\partial x}+\frac{\partial B_a^{*}}{\partial h}\frac{\partial h}{\partial x} \tag{3.4}$$

$$\frac{\partial A}{\partial t} = B_t\frac{\partial h}{\partial t} = \left[B_a^{*}+h\frac{\partial B_a^{*}}{\partial h}\right]\frac{\partial h}{\partial t} \tag{3.5}$$

and assume

$$\frac{\partial F_x}{\partial x} = \frac{\partial}{\partial x}\left[\nu A\frac{\partial u}{\partial x}\right] = \frac{\partial}{\partial x}\left[\nu B_a h\frac{\partial u}{\partial x}\right] \tag{3.6}$$

where ν is the eddy viscosity coefficient [L^2/T]; $B_t(XT)$ ($= B_t^{*}(x,h(XT))$) is the top river/stream width [L]; $B_a(XT)$ ($= B_a^{*}(x,h(XT))$) is the average river/stream width [L]. Thus, Eqs. (3.1) and (3.2) can

be rewritten as follows after letting $H = h + Z_0$ and some mathematical manipulation.

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} + \frac{hB_a}{B_t}\frac{\partial u}{\partial x} = \frac{1}{B_t}(S_S + S_R - S_I + S_1 + S_2) - \frac{uh}{B_t}\frac{\partial B_a^*}{\partial x} + u\frac{\partial Z_0}{\partial x} \tag{3.7}$$

$$\begin{aligned}\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + g\frac{\partial H}{\partial x} &= \frac{1}{hB_a}\frac{\partial}{\partial x}\left[\nu B_a h\frac{\partial u}{\partial x}\right] \\ &+ \frac{1}{hB_a}\left[-uS_S + (u^r - u)S_R - (u^i - u)S_I + (u^{Y1} - u)S_1 + (u^{Y2} - u)S_2 + \frac{T^s - T^b}{\rho}\right]\end{aligned} \tag{3.8}$$

Thus, Eqs. (3.7) and (3.8) can be written in matrix form as

$$\frac{\partial E}{\partial t} + A\frac{\partial E}{\partial x} = R \tag{3.9}$$

where

$$E = \{H \quad u\}^T \tag{3.10}$$

$$A = \begin{bmatrix} u & \frac{hB_a}{B_t} \\ g & u \end{bmatrix} \tag{3.11}$$

and

$$R = \{R_1 \quad R_2\}^T \tag{3.12}$$

in which

$$R_1 = \frac{1}{B_t}(S_S + S_R - S_I + S_1 + S_2) - \frac{uh}{B_t}\frac{\partial B_a^*}{\partial x} + u\frac{\partial Z_0}{\partial x} \tag{3.13}$$

$$\begin{aligned}R_2 &= \frac{1}{hB_a}\frac{\partial}{\partial x}\left[\nu B_a h\frac{\partial u}{\partial x}\right] \\ &+ \frac{1}{hB_a}\left[-uS_S + (u^r - u)S_R - (u^i - u)S_I + (u^{Y1} - u)S_1 + (u^{Y2} - u)S_2 + \frac{T^s - T^b}{\rho}\right]\end{aligned} \tag{3.14}$$

Eq. (3.9) can be written as

$$\frac{\partial E}{\partial t} + A^d\frac{\partial E}{\partial x} = RJ + RD \tag{3.15}$$

where

$$A^d = \begin{bmatrix} u & 0 \\ 0 & u \end{bmatrix} \tag{3.16}$$

and

$$RD = \begin{Bmatrix} RD_1 \\ RD_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ \frac{1}{hB_a}\frac{\partial}{\partial x}\left(hB_a \nu \frac{\partial u}{\partial x} \right) \end{Bmatrix} \tag{3.17}$$

$$RJ = \begin{Bmatrix} RJ_1 \\ RJ_2 \end{Bmatrix} = \begin{Bmatrix} R_1 - \frac{hB_a}{B_t}\frac{\partial u}{\partial x} \\ R_2 - RD_2 - g\frac{\partial H}{\partial x} \end{Bmatrix} \tag{3.18}$$

Eq. (3.15) can be further written as

$$\frac{DE}{Dt} = RJ + RD \tag{3.19}$$

where

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A^d \frac{\partial E}{\partial x} \tag{3.20}$$

Let $E^{\#}$ be the solution of

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A^d \frac{\partial E}{\partial x} = RJ \tag{3.21}$$

We have, from Eq. (3.19)

$$\frac{E - E^p}{\Delta t} = RJ + RD \tag{3.22}$$

where E^p represents the Lagrangian value of E. From Eq. (3.21)

$$\frac{E^{\#} - E^p}{\Delta t} = RJ \tag{3.23}$$

Subtracting Eq. (3.23) from Eq. (3.22) yields

$$\frac{E - E^{\#}}{\Delta t} = RD \tag{3.24}$$

Based on the above, we mean to solve Eq. (3.21) for $E^{\#}$ at first and solve Eq. (3.24) for E based on $E^{\#}$. Eq. (3.21) is solved by the method of characteristics as follows.

Eq. (3.21) can be written as

$$\frac{\partial E}{\partial t} + A\frac{\partial E}{\partial x} = RI \tag{3.25}$$

where

$$RJ = \begin{Bmatrix} RI_1 \\ RI_2 \end{Bmatrix} = \begin{Bmatrix} R_1 \\ R_2 - RD_2 \end{Bmatrix} \tag{3.26}$$

The eigenvalues and eigenvectors of A are

$$\lambda_1 = u + \sqrt{\frac{ghB_a}{B_t}} \qquad e_1 = \left\{ \frac{1}{2}\sqrt{\frac{hB_a}{gB_t}} \quad \frac{1}{2} \right\}^T \tag{3.27}$$

$$\lambda_1 = u - \sqrt{\frac{ghB_a}{B_t}} \qquad e_1 = \left\{ -\frac{1}{2}\sqrt{\frac{hB_a}{gB_t}} \quad \frac{1}{2} \right\}^T \tag{3.28}$$

Now, we define

$$L = \begin{bmatrix} \frac{c}{2g} & -\frac{c}{2g} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \tag{3.29}$$

Thus

$$L^{-1} = \begin{bmatrix} \frac{g}{c} & 1 \\ -\frac{g}{c} & 1 \end{bmatrix} \tag{3.30}$$

Set

$$\partial W = L^{-1}\partial E = \begin{bmatrix} \frac{g}{c} & 1 \\ -\frac{g}{c} & 1 \end{bmatrix} \begin{Bmatrix} \partial H \\ \partial u \end{Bmatrix} \tag{3.31}$$

Multiplying both side of Eq. (3.25) by L^{-1} yields

$$L^{-1}\frac{\partial E}{\partial t} + L^{-1}ALL^{-1}\frac{\partial E}{\partial x} = L^{-1}RI \tag{3.32}$$

or

$$\frac{\partial W}{\partial t} + \begin{bmatrix} u+c & 0 \\ 0 & u-c \end{bmatrix} \frac{\partial W}{\partial x} = L^{-1}RI \tag{3.33}$$

or

$$\frac{DW}{Dt} = L^{-1}RI \tag{3.34}$$

where

$$c = \sqrt{\frac{ghB_a}{B_t}} \tag{3.35}$$

Eq. (3.34) can be discretized, in time, as follows.

$$\frac{g}{c}\frac{H^{n+1}-H_1^*}{\Delta\tau_1} + \frac{u^{n+1}-u_1^*}{\Delta\tau_1} = \frac{g}{c}RI_1 + RI_2 \tag{3.36}$$

$$\frac{-g}{c}\frac{H^{n+1}-H_2^*}{\Delta\tau_2} + \frac{u^{n+1}-u_2^*}{\Delta\tau_2} = \frac{-g}{c}RI_1 + RI_2 \tag{3.37}$$

where H_1^*, u_1^*, and $\Delta\tau_1$ are determined by backward tracking along the first characteristic; H_2^*, u_2^*, and $\Delta\tau_2$ are determined by backward tracking along the second characteristic.

Backward tracking along characteristics for 1-D channel flow

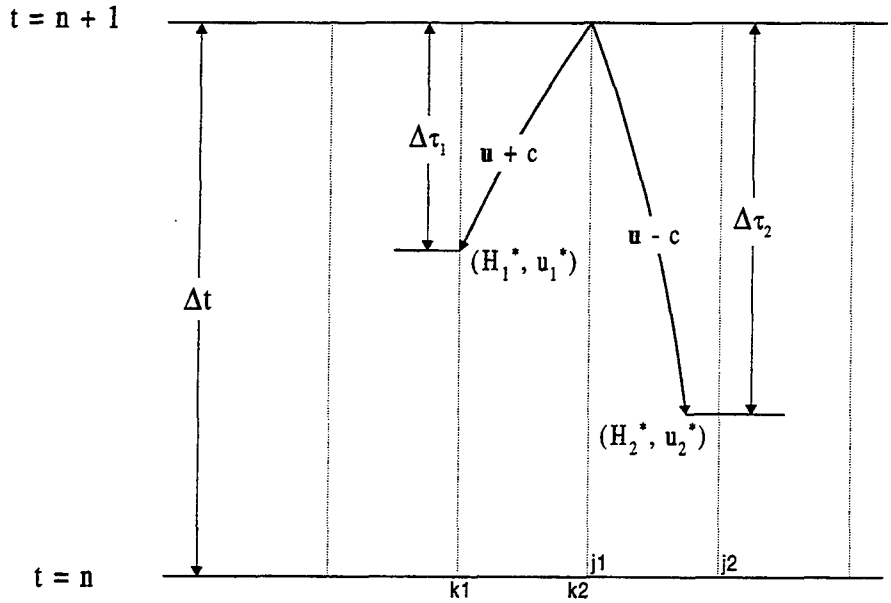

Figure 3.1. Tracking along characteristics in solving 1-D dynamic wave equation.

and

$$H_1^* = a_1 H_{k1}^{n+1} + a_2 H_{k2}^{n+1} + a_3 \tag{3.38}$$

$$u_1^* = a_1 u_{k1}^{n+1} + a_2 u_{k2}^{n+1} + a_4 \tag{3.39}$$

$$H_2^* = b_1 H_{j1}^{n+1} + b_2 H_{j2}^{n+1} + b_3 \tag{3.40}$$

$$u_2^* = b_1 u_{j1}^{n+1} + b_2 u_{j2}^{n+1} + b_4 \tag{3.41}$$

in which k1 and k2 are nodes of the element that the backward tracking, along the first characteristic, stops in; j1 and j2 are nodes of the element that the backward tracking, along the second characteristic, stops in. (see the above figure)

Note: 1. a_1, a_2, b_1, and b_2 are within the range of [0,1].
2. We may use two given parameters to determine where to stop in the backward tracking: one is for controlling tracking time and the other one is for controlling tracking distance.

Multiplying Eqs. (3.36) and (3.37) with cross-sectional area yields

$$\frac{ghB_a}{c\Delta\tau_1}\left(H - H_1^*\right) + \frac{hB_a}{\Delta\tau_1}\left(u - u_1^*\right) + hB_a\left[\frac{c}{B_t}\frac{\partial B_a^*}{\partial x} - \frac{g}{c}\frac{\partial Z_0}{\partial x}\right]u + \left(Ph\kappa + S_S + S_R - S_I + S_1 + S_2\right)u$$
$$= \frac{ghB_a}{cB_t}\left(S_S + S_R - S_I + S_1 + S_2\right) + \left(u^r S_R - u^i S_I + u^{Y1} S_1 + u^{Y2} S_2\right) + \frac{B_t \tau^s}{\rho} + \frac{\partial}{\partial x}\left(\nu h B_a \frac{\partial u}{\partial x}\right) \tag{3.42}$$

$$\frac{-ghB_a}{c\Delta\tau_2}\left(H - H_2^*\right) + \frac{hB_a}{\Delta\tau_2}\left(u - u_2^*\right) - hB_a\left[\frac{c}{B_t}\frac{\partial B_a^*}{\partial x} - \frac{g}{c}\frac{\partial Z_0}{\partial x}\right]u + \left(Ph\kappa + S_S + S_R - S_I + S_1 + S_2\right)u$$
$$= -\frac{ghB_a}{cB_t}\left(S_S + S_R - S_I + S_1 + S_2\right) + \left(u^r S_R - u^i S_I + u^{Y1} S_1 + u^{Y2} S_2\right) + \frac{B_t \tau^s}{\rho} + \frac{\partial}{\partial x}\left(\nu h B_a \frac{\partial u}{\partial x}\right) \tag{3.43}$$

In obtaining Eqs. (3.42) and (3.43), the following relationships have been employed.

$$\frac{T^b}{\rho} = Ph\kappa u \tag{3.44}$$

$$\frac{T^s}{\rho} = \frac{B_t \tau^s}{\rho} \tag{3.45}$$

When H_1^*, u_1^*, H_2^*, and u_2^* are determined explicitly by using the spatial reach out option in backward tracking (i.e., track backward all the way to the previous time), Eqs. (3.42) and (3.43) can be solved for ($H^\#$, $u^\#$) node by node as follows.

Eqs. (3.42) and (3.43), after multiplied by $\Delta\tau_1$ and $\Delta\tau_2$, respectively, can be written as

$$a_{11} H + a_{12} u = b_1 \tag{3.46}$$

$$a_{21}H + a_{22}u = b_2 \tag{3.47}$$

where

$$a_{11} = cB_a \tag{3.48}$$

$$a_{22} = hB_a\left[1 + \left(\frac{c}{B_t}\frac{\partial B_a^*}{\partial x} - \frac{g}{c}\frac{\partial Z_0}{\partial x}\right)\Delta\tau_1\right] + \left(Ph\kappa + S_S + S_R - S_I + S_1 + S_2\right)\Delta\tau_1 \tag{3.49}$$

$$b_1 = cB_aH_1^* + hB_au_1^*$$
$$+\frac{cB_a\Delta\tau_1}{B_t}\left(S_S + S_R - S_I + S_1 + S_2\right) + \Delta\tau_1\left(u^rS_R - u^iS_I + u^{Y1}S_1 + u^{Y2}S_2\right) + \frac{B_t\tau^s\Delta\tau_1}{\rho} \tag{3.50}$$

$$a_{21} = -cB_a \tag{3.51}$$

$$a_{22} = hB_a\left[1 - \left(\frac{c}{B_t}\frac{\partial B_a^*}{\partial x} - \frac{g}{c}\frac{\partial Z_0}{\partial x}\right)\Delta\tau_2\right] + \left(Ph\kappa + S_S + S_R - S_I + S_1 + S_2\right)\Delta\tau_2 \tag{3.52}$$

$$b_2 = -cB_aH_2^* + hB_au_2^*$$
$$-\frac{cB_a\Delta\tau_2}{B_t}\left(S_S + S_R - S_I + S_1 + S_2\right) + \Delta\tau_2\left(u^rS_R - u^iS_I + u^{Y1}S_1 + u^{Y2}S_2\right) + \frac{B_t\tau^s\Delta\tau_2}{\rho} \tag{3.53}$$

Therefore, we solve Eqs. (3.46) and (3.47) for $H^{\#}$ and $u^{\#}$. Now, we can solve Eq. (3.24) as follows. Eq. (3.24) can be written in details as

$$\frac{H - H^{\#}}{\Delta t} = 0 \tag{3.54}$$

$$\frac{hB_a(u - u^{\#})}{\Delta t} = \frac{\partial}{\partial x}\left(\nu hB_a\frac{\partial u}{\partial x}\right) \tag{3.55}$$

Eq. (3.54) gives that $H = H^{\#}$, while Eq. (3.55) can be discretized, in the finite element method, as

$$\frac{hB_a}{\Delta t}[QA]\{u\} + [QD]\{u\} = \{QR\} + \{BQ\} \tag{3.56}$$

where

$$QA_{i,j} = \sum_{e\in M_e}\int_{R_e} N_\alpha^e N_\beta^e\, dR \tag{3.57}$$

$$QD_{i,j} = \sum_{e \in M_e} \int_{R_e} \nabla N_\alpha^e \, h \nu B_a \nabla N_\beta^e \, dR \tag{3.58}$$

$$QR_i = \sum_{e \in M_e} \int_{R_e} N_\alpha^e \frac{hB_a u^\#}{\Delta t} dR \tag{3.59}$$

$$BQ_i = \sum_{e \in M_e} \int_{B_e} N_\alpha^e \, n h B_a \frac{\partial u}{\partial x} dB \tag{3.60}$$

in Eq. (3.60), n = -1 for upstream boundary nodes while n = 1 for downstream boundary nodes.

In solving Eqs. (3.42) and (3.43) at boundary nodes, boundary conditions are implemented as follows. A boundary node can be either an closed or an open (flow-through) boundary. In the former case, nothing is specified and velocity at the node is set to zero automatically in the computer code. While in the latter case, H, and u of the approaching flow, with respect to the characteristic ongoing direction, must be given at the boundary nodes. Some details are given for both cases below.

< Case 1 > Closed boundaries: If the closed boundary is located at the downstream end, only sub-critical flow can happen because the velocity is zero. Under this condition, one characteristic comes from the outside of the domain and the other one is from the inside. The equation associated with the characteristic from outside will be replaced by u = 0, while the other (either Eq. (3.40) or (3.41)) is used for the other characteristic. On the other hand, if the closed boundary is located at the upstream end, either sub-critical or super-critical flow can occur. If the flow is sub-critical, again, the equation associated with the characteristic from outside will be replaced by u = 0, while the other (either Eq. (3.40) or (3.41)) is used for the other characteristic. If the flow is super-critical then both u and h are set to zero.

< Case 2 > Open boundaries: In this case, three types of boundary conditions can be given for sub-critical flow when the propagation direction of a characteristic is inward to the domain of interest. They are described as follows.

(1) Given time-dependent flow rate, Q(t): (used for upstream open boundaries)

$$\mathbf{n} \cdot \mathbf{u} = \frac{Q}{hB_a} = \frac{Q}{A} \tag{3.61}$$

(2) Given time-dependent water stage, $H_b(t)$: (used for either upstream or downstream open boundaries)

$$H = H_b \tag{3.62}$$

(3) Given rating water depth-dependent flow rate, Q(h): (used for natural downstream open boundaries only)

$$\mathbf{n}\cdot\mathbf{u} = \frac{Q}{hB_a} = \frac{Q}{A} \tag{3.63}$$

On the other hand, for super-critical flow either no boundary conditions is required when the open boundary is located downstream, or both u and h must be prescribed when the open boundary is located upstream.

3.1.2. The Lagrangian approach for both 1-D diffusion and 1-D kinematic wave models

Since the kinematic wave model can be considered to be a simplified form from a mathematical point of view, we just demonstrate how the diffusion wave equations are solved with the Lagranging approach in the following. Its application to solving the kinematic wave equations is straightforward.

Recall Eqs. (2.1) and (2.3)

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = S_S + S_R - S_I + S_1 + S_2 \tag{3.64}$$

$$u = \frac{-1}{n}\left[\frac{R}{1+(\nabla Z_0)^2}\right]^{2/3} \frac{1}{(\nabla(Z_0+h))^{1/2}} \frac{\partial(Z_0+h)}{\partial x} \tag{3.65}$$

Eq. (3.64) can be further written as

$$B_t \frac{\partial h}{\partial t} + \frac{\partial(uhB_a)}{\partial x} = S_S + S_R - S_I + S_1 + S_2 \tag{3.66}$$

Substituting Eq.(3.65) into the second term on the left side of Eq. (3.66) yields

$$\frac{\partial huB_a}{\partial x} = uB_a \frac{\partial h}{\partial x} + uh\frac{\partial B_a}{\partial x} + hB_a \frac{\partial u}{\partial x} = \left(uB_a + uh\frac{\partial B^*}{\partial h} + hB_a \frac{2}{3}\frac{u}{R}\frac{\partial R^*}{\partial h}\right)\frac{\partial h}{\partial x} + S \tag{3.67}$$

where

$$S = \frac{-hB_a}{n}\frac{R^{2/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{1}{(\nabla(Z_0+h))^{1/2}}\frac{\partial^2(Z_0+h)}{\partial x^2}+\frac{hB_a}{n^2}\frac{R^{2/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{1}{(\nabla Z_0)^{1/2}}\frac{\partial(Z_0+h)}{\partial x}\frac{\partial n}{\partial x}$$

$$+\frac{-hB_a}{n}\frac{R^{2/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{\partial Z_0}{\partial x}\frac{-1}{4}\left[\left(\frac{\partial(Z_0+h)}{\partial x}\right)^2\right]^{-5/4}2\left[\frac{\partial(Z_0+h)}{\partial x}\frac{\partial^2(Z_0+h)}{\partial x^2}\right]$$

$$+\frac{-hB_a}{n}\left[\frac{1}{1+(\nabla Z_0)^2}\right]^{2/3}\frac{1}{(\nabla(Z_0+h))^{1/2}}\frac{\partial(Z_0+h)}{\partial x}\frac{2}{3}R^{-1/3}\frac{\partial R^*}{\partial x} \qquad (3.68)$$

$$+\frac{-hB_a}{n}\frac{R^{2/3}}{(\nabla(Z_0+h))^{1/2}}\frac{\partial(Z_0+h)}{\partial x}\frac{-2}{3}\left[1+(\nabla Z_0)^2\right]^{-5/3}2\left[\frac{\partial Z_0}{\partial x}\frac{\partial^2 Z_0}{\partial x^2}\right]+hu\frac{\partial B_a^*}{\partial x}$$

Therefore, Eq. (3.66) can be written as

$$B_t\frac{\partial h}{\partial t}+\left(uB_a+uh\frac{\partial B^*}{\partial h}+hB_a\frac{2}{3}\frac{u}{R}\frac{\partial R^*}{\partial h}\right)\frac{\partial h}{\partial x} = S_S+S_R-S_I+S_1+S_2-S \qquad (3.69)$$

Eq. (3.69) can be further written as

$$B_t\frac{Dh}{Dt} = S_S+S_R-S_I+S_1+S_2-S \qquad (3.70)$$

where the following characteristic equation applies.

$$\frac{dx}{dt} = \frac{uB_a+uh\frac{\partial B^*}{\partial h}+hB_a\frac{2}{3}\frac{u}{R}\frac{\partial R^*}{\partial h}}{B_t} \qquad (3.71)$$

Hence the solution to Eq. (3.69) is

$$h(x,t) = h(x_0,0)+(S_S+S_R-S_I+S_1+S_2-S)t \qquad (3.72)$$

in which

$$x-x_0 = \int_0^t \frac{uB_a+uh\frac{\partial B^*}{\partial h}+hB_a\frac{2}{3}\frac{u}{R}\frac{\partial R^*}{\partial h}}{B_t}dt \qquad (3.73)$$

A nonlinear iteration loop with the Picard method implemented is used to solve Eqs. (3.7) and (3.8) in the dynamic wave model or to solve Eqs. (3.64) and (3.65) in the diffusion wave model during each time step.

3.1.3. Computation of water budget at junctions

In the model, a junction is considered to be a reservoir and water budget is used to determine the water stage there. Thus, the governing equation to compute water stage at a junction can be

written as

$$\frac{dV_j}{dt} = \sum_{i=1}^{ncr} Q_i \tag{3.74}$$

where V_j is the volume of water at the junction [L^3]; Q_i is the flow rate associated with the junction's i-th connected river/stream reach [L^3/T]; ncr is the number of river/stream reaches that is connected to the junction. Since V_j can be expressed as a function of water depth at the junction, the stage at the junction can be determined once V_j is computed. In our model, Eq. (3.74) is solved implicitly (i.e., within the nonlinear iteration loop).

3.2. Solving the 2-D overland flow equations

3.2.1. Method of characteristics for 2-D dynamic wave model

Recall Eqs. (2.9) through (2.11)

$$\frac{\partial h}{\partial t} + \frac{\partial uh}{\partial x} + \frac{\partial vh}{\partial y} = SS + R - I \tag{3.75}$$

$$\frac{\partial uh}{\partial t} + \frac{\partial u^2 h}{\partial x} + \frac{\partial uvh}{\partial y} = -gh\frac{\partial (Z_0 + h)}{\partial x} + \frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y} + (u^r R - u^i I) + \frac{\tau_x^s - \tau_x^b}{\rho} \tag{3.76}$$

$$\frac{\partial vh}{\partial t} + \frac{\partial uvh}{\partial x} + \frac{\partial v^2 h}{\partial y} = -gh\frac{\partial (Z_0 + h)}{\partial y} + \frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y} + (v^r R - v^i I) + \frac{\tau_y^s - \tau_y^b}{\rho} \tag{3.77}$$

Let $H=h+Z_0$, then Eqs. (3.75) through (3.77) can be written as follows after mathematical manipulation.

$$\frac{\partial H}{\partial t} + u\frac{\partial H}{\partial x} + h\frac{\partial u}{\partial x} + v\frac{\partial H}{\partial y} + h\frac{\partial v}{\partial y} = (SS + R - I) + u\frac{\partial Z_0}{\partial x} + v\frac{\partial Z_0}{\partial y} \tag{3.78}$$

$$\frac{\partial u}{\partial t} + g\frac{\partial H}{\partial x} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \frac{1}{h}\left[\frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y}\right] + \frac{(u^r - u)R - (u^i - u)I}{h} + \frac{\tau_x^s - \tau_x^b}{h\rho} - \frac{SS\,u}{h} \tag{3.79}$$

$$\frac{\partial v}{\partial t} + g\frac{\partial H}{\partial y} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = \frac{1}{h}\left[\frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y}\right] + \frac{(v^r - v)R - (v^i - v)I}{h} + \frac{\tau_y^s - \tau_y^b}{h\rho} - \frac{SS\,v}{h} \tag{3.80}$$

Thus, Eqs. (3.78) through (3.80) can be written in matrix form as

$$\frac{\partial E}{\partial t} + A_x\frac{\partial E}{\partial x} + A_y\frac{\partial E}{\partial y} = R \tag{3.81}$$

where

$$E = \{H \;\; u \;\; v\}^T \tag{3.82}$$

$$A_x = \begin{bmatrix} u & h & 0 \\ g & u & 0 \\ 0 & 0 & u \end{bmatrix} \qquad A_y = \begin{bmatrix} v & 0 & h \\ 0 & v & 0 \\ g & 0 & v \end{bmatrix} \tag{3.83}$$

and

$$R = \begin{Bmatrix} R_1 \\ R_2 \\ R_3 \end{Bmatrix} = \begin{Bmatrix} SS + R - I + u\dfrac{\partial Z_0}{\partial x} + v\dfrac{\partial Z_0}{\partial y} \\ \dfrac{1}{h}\left[\dfrac{\partial F_{xx}}{\partial x} + \dfrac{\partial F_{yx}}{\partial y}\right] + \dfrac{(u^r - u)R - (u^i - u)I}{h} + \dfrac{\tau_x^s - \tau_x^b}{h\rho} - \dfrac{SS\,u}{h} \\ \dfrac{1}{h}\left[\dfrac{\partial F_{xy}}{\partial x} + \dfrac{\partial F_{yy}}{\partial y}\right] + \dfrac{(v^r - v)R - (v^i - v)I}{h} + \dfrac{\tau_y^s - \tau_y^b}{h\rho} - \dfrac{SS\,v}{h} \end{Bmatrix} \tag{3.84}$$

By using the splitting strategy mentioned in Section 3.1.1, Eq. (3.81) can be written as

$$\frac{\partial E}{\partial t} + A_x^d \frac{\partial E}{\partial x} + A_y^d \frac{\partial E}{\partial y} = RJ + RD \tag{3.85}$$

where

$$A_x^d = \begin{bmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{bmatrix} \qquad A_y^d = \begin{bmatrix} v & 0 & 0 \\ 0 & v & 0 \\ 0 & 0 & v \end{bmatrix} \tag{3.86}$$

and

$$RD = \begin{Bmatrix} RD_1 \\ RD_2 \\ RD_3 \end{Bmatrix} = \begin{Bmatrix} 0 \\ \dfrac{1}{h}\left[\dfrac{\partial F_{xx}}{\partial x} + \dfrac{\partial F_{yx}}{\partial y}\right] \\ \dfrac{1}{h}\left[\dfrac{\partial F_{xy}}{\partial x} + \dfrac{\partial F_{yy}}{\partial y}\right] \end{Bmatrix} \tag{3.87}$$

$$RJ = \begin{Bmatrix} RJ_1 \\ RJ_2 \\ RJ_3 \end{Bmatrix} = \begin{Bmatrix} R_1 - h\dfrac{\partial u}{\partial x} - h\dfrac{\partial v}{\partial y} \\ R_2 - RD_2 - g\dfrac{\partial H}{\partial x} \\ R_3 - RD_3 - g\dfrac{\partial H}{\partial y} \end{Bmatrix} \tag{3.88}$$

Eq. (3.85) can be further written as

$$\frac{DE}{Dt} = RJ + RD \tag{3.89}$$

where

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A_x^{\,d}\frac{\partial E}{\partial x} + A_y^{\,d}\frac{\partial E}{\partial y} \tag{3.90}$$

Let $E^{\#}$ be the solution of

$$\frac{DE}{Dt} = \frac{\partial E}{\partial t} + A_x^{\,d}\frac{\partial E}{\partial x} + A_y^{\,d}\frac{\partial E}{\partial y} = RJ \tag{3.91}$$

we have, from Eq. (3.89)

$$\frac{E - E^{p}}{\Delta t} = RJ + RD \tag{3.92}$$

where E^p represents the Lagrangian value of E. From Eq. (3.91)

$$\frac{E^{\#} - E^{p}}{\Delta t} = RJ \tag{3.93}$$

Subtracting Eq. (3.93) from Eq. (3.92) yields

$$\frac{E - E^{\#}}{\Delta \tau} = RD \tag{3.94}$$

Based on the above, we mean to solve Eq. (3.93) for $E^{\#}$ at first and solve Eq. (3.94) for E based on $E^{\#}$. Eq. (3.93) is to be solved by the method of characteristics and can be written, in details, as follows.

Eq. (3.93) can be written as

$$\frac{\partial E}{\partial t} + A_x\frac{\partial E}{\partial x} + A_y\frac{\partial E}{\partial y} = RI \tag{3.95}$$

where

$$RI = \begin{Bmatrix} RI_1 \\ RI_2 \\ RI_3 \end{Bmatrix} = \begin{Bmatrix} R_1 \\ R_2 - RD_2 \\ R_3 - RD_3 \end{Bmatrix} \tag{3.96}$$

Let

$$\mathbf{A}\cdot\mathbf{k} = A_x k_x + A_y k_y = \begin{bmatrix} uk_x + vk_y & hk_x & hk_y \\ gk_x & uk_x + vk_y & 0 \\ gk_y & 0 & uk_x + vk_y \end{bmatrix} \tag{3.97}$$

the associated eigenvalues and eigenvectors are

$$\lambda_1 = uk_x + vk_y \qquad e_1 = \{0 \;\; k_y \;\; -k_x\}^T \tag{3.98}$$

$$\lambda_2 = uk_x + vk_y + \sqrt{gh} \qquad e_2 = \left\{ \frac{\sqrt{gh}}{2} \quad \frac{gk_x}{2} \quad \frac{gk_y}{2} \right\}^T \tag{3.99}$$

$$\lambda_3 = uk_x + vk_y - \sqrt{gh} \qquad e_3 = \left\{ -\frac{\sqrt{gh}}{2} \quad \frac{gk_x}{2} \quad \frac{gk_y}{2} \right\}^T \tag{3.100}$$

Now, we define

$$L = \begin{bmatrix} 0 & \frac{\sqrt{gh}}{2} & -\frac{\sqrt{gh}}{2} \\ k_y & \frac{gk_x}{2} & \frac{gk_x}{2} \\ -k_x & \frac{gk_y}{2} & \frac{gk_y}{2} \end{bmatrix} \tag{3.101}$$

Thus

$$L^{-1} = \begin{bmatrix} 0 & k_y & -k_x \\ \frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \\ -\frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \end{bmatrix} \tag{3.102}$$

Let

$$\partial W = L^{-1}\partial E = \begin{bmatrix} 0 & k_y & -k_x \\ \frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \\ -\frac{1}{\sqrt{gh}} & \frac{k_x}{g} & \frac{k_y}{g} \end{bmatrix} \begin{Bmatrix} \partial H \\ \partial u \\ \partial v \end{Bmatrix} \tag{3.103}$$

and multiply both sides of Eq. (3.95) by L^{-1}. Thus, we obtain

$$L^{-1}\frac{\partial E}{\partial t} + L^{-1}A_x L L^{-1}\frac{\partial E}{\partial x} + L^{-1}A_y L L^{-1}\frac{\partial E}{\partial y} = L^{-1}RI \tag{3.104}$$

or

$$\frac{\partial W}{\partial t} + L^{-1}A_x L\frac{\partial W}{\partial x} + L^{-1}A_y L\frac{\partial W}{\partial y} = L^{-1}RI \tag{3.105}$$

or

$$\frac{\partial W}{\partial t}+\begin{bmatrix} u & \frac{gck_y}{2} & -\frac{gck_y}{2} \\ \frac{hk_y}{c} & u+ck_x & 0 \\ -\frac{hk_y}{c} & 0 & u-ck_x \end{bmatrix}\frac{\partial W}{\partial x}+\begin{bmatrix} v & -\frac{gck_x}{2} & \frac{gck_x}{2} \\ -\frac{hk_x}{c} & v+ck_y & 0 \\ \frac{hk_x}{c} & 0 & v-ck_y \end{bmatrix}\frac{\partial W}{\partial y} = L^{-1}RI \qquad (3.106)$$

where

$$c = \sqrt{gh} \qquad (3.107)$$

After arrangement, Eq. (3.106) can be rewritten as follows.

$$\frac{\partial W}{\partial t}+\begin{bmatrix} u & 0 & 0 \\ 0 & u+ck_x & 0 \\ 0 & 0 & u-ck_x \end{bmatrix}\frac{\partial W}{\partial x}+\begin{bmatrix} v & 0 & 0 \\ 0 & v+ck_y & 0 \\ 0 & 0 & v-ck_y \end{bmatrix}\frac{\partial W}{\partial y}$$

$$+\begin{Bmatrix} g\left(k_y\frac{\partial H}{\partial x}-k_x\frac{\partial H}{\partial y}\right) \\ \frac{h}{c}\left[k_yk_y\frac{\partial u}{\partial x}+k_xk_x\frac{\partial v}{\partial y}-k_xk_y\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right] \\ \frac{-h}{c}\left[k_yk_y\frac{\partial u}{\partial x}+k_xk_x\frac{\partial v}{\partial y}-k_xk_y\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right] \end{Bmatrix} = L^{-1}RI \qquad (3.108)$$

For a general consideration, we define a new L^{-1} which plays the following transformation.

$$\partial W = L^{-1}\partial E = \begin{bmatrix} 0 & k_y^{(1)} & -k_x^{(1)} \\ \frac{1}{c} & \frac{k_x^{(2)}}{g} & \frac{k_y^{(2)}}{g} \\ -\frac{1}{c} & \frac{k_x^{(2)}}{g} & \frac{k_y^{(2)}}{g} \end{bmatrix}\begin{Bmatrix} \partial H \\ \partial u \\ \partial v \end{Bmatrix} \qquad (3.109)$$

Multiplying both side of Eq. (3.95) by this new L^{-1} and repeating mathematical manipulations involved in Eqs. (3.106) and (3.108) yields

$$\frac{\partial W}{\partial t}+\begin{bmatrix} u & 0 & 0 \\ 0 & u+ck_x^{(2)} & 0 \\ 0 & 0 & u-ck_x^{(2)} \end{bmatrix}\frac{\partial W}{\partial x}+\begin{bmatrix} v & 0 & 0 \\ 0 & v+ck_y^{(2)} & 0 \\ 0 & 0 & v-ck_y^{(2)} \end{bmatrix}\frac{\partial W}{\partial y}$$

$$+\begin{Bmatrix} g\left(k_y^{(1)}\frac{\partial H}{\partial x}-k_x^{(1)}\frac{\partial H}{\partial y}\right) \\ \frac{h}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x}+k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y}-k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right] \\ \frac{-h}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x}+k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y}-k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right] \end{Bmatrix} = L^{-1}RI \tag{3.110}$$

or

$$\begin{Bmatrix} \frac{DW_1}{Dt} \\ \frac{DW_2}{Dt} \\ \frac{DW_3}{Dt} \end{Bmatrix}+\begin{Bmatrix} S_1 \\ S_2 \\ S_3 \end{Bmatrix}=\begin{Bmatrix} k_y^{(1)}RI_2-k_x^{(1)}RI_3 \\ \frac{1}{c}RI_1+\frac{k_x^{(2)}}{g}RI_2+\frac{k_y^{(2)}}{g}RI_3 \\ \frac{-1}{c}RI_1+\frac{k_x^{(2)}}{g}RI_2+\frac{k_y^{(2)}}{g}RI_3 \end{Bmatrix} \tag{3.111}$$

where

$$\frac{DW_1}{Dt}=\frac{\partial W_1}{\partial t}+u\frac{\partial W_1}{\partial x}+v\frac{\partial W_1}{\partial y} \tag{3.112}$$

$$\frac{DW_2}{Dt}=\frac{\partial W_2}{\partial t}+\left(u+ck_x^{(2)}\right)\frac{\partial W_2}{\partial x}+\left(v+ck_y^{(2)}\right)\frac{\partial W_2}{\partial y} \tag{3.113}$$

$$\frac{DW_3}{Dt}=\frac{\partial W_3}{\partial t}+\left(u-ck_x^{(2)}\right)\frac{\partial W_3}{\partial x}+\left(v-ck_y^{(2)}\right)\frac{\partial W_3}{\partial y} \tag{3.114}$$

$$S_1=g\left(k_y^{(1)}\frac{\partial H}{\partial x}-k_x^{(1)}\frac{\partial H}{\partial y}\right) \tag{3.115}$$

$$S_2=\frac{h}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x}+k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y}-k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right] \tag{3.116}$$

$$S_3=\frac{-h}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x}+k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y}-k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right] \tag{3.117}$$

Note: Diagonalization can be achieved under special selections of $k_x^{(1)}$, $k_y^{(1)}$, $k_x^{(2)}$, and $k_y^{(2)}$ to make zeros of S_1, S_2, and S_3.

Eq. (3.107) can be discretized, in time, as follows.

$$k_y^{(1)}\frac{u^{n+1}-u_1^*}{\Delta\tau_1}-k_x^{(1)}\frac{v^{n+1}-v_1^*}{\Delta\tau_1}+S_1 = k_y^{(1)}RI_2-k_x^{(1)}RI_3 \tag{3.118}$$

$$\frac{1}{c}\frac{H^{n+1}-H_2^*}{\Delta\tau_2}+\frac{k_x^{(2)}}{g}\frac{u^{n+1}-u_2^*}{\Delta\tau_2}+\frac{k_y^{(2)}}{g}\frac{v^{n+1}-v_2^*}{\Delta\tau_2}+S_2 = \frac{1}{c}RI_1+\frac{k_x^{(2)}}{g}RI_2+\frac{k_y^{(2)}}{g}RI_3 \tag{3.119}$$

$$\frac{-1}{c}\frac{H^{n+1}-H_3^*}{\Delta\tau_3}+\frac{k_x^{(2)}}{g}\frac{u^{n+1}-u_3^*}{\Delta\tau_3}+\frac{k_y^{(2)}}{g}\frac{v^{n+1}-v_3^*}{\Delta\tau_3}+S_3 = \frac{-1}{c}RI_1+\frac{k_x^{(2)}}{g}RI_2+\frac{k_y^{(2)}}{g}RI_3 \tag{3.120}$$

where u_1^*, v_1^*, and $\Delta\tau_1$ are determined by backward tracking along the first characteristic; H_2^*, u_2^*, v_2^*, and $\Delta\tau_2$ are determined by backward tracking along the second characteristic; H_3^*, u_3^*, v_3^*, and $\Delta\tau_3$ are determined by backward tracking along the third characteristic; and

$$u_1^* = a_1u_{k1}^{n+1}+a_2u_{k2}^{n+1}+a_3u_{k3}^{n+1}+a_4u_{k4}^{n+1}+a_6 \tag{3.121}$$

$$v_1^* = a_1v_{k1}^{n+1}+a_2v_{k2}^{n+1}+a_3v_{k3}^{n+1}+a_4v_{k4}^{n+1}+a_7 \tag{3.122}$$

$$H_2^* = b_1H_{j1}^{n+1}+b_2H_{j2}^{n+1}+b_3H_{j3}^{n+1}+b_4H_{j4}^{n+1}+b_5 \tag{3.123}$$

$$u_2^* = b_1u_{j1}^{n+1}+b_2u_{j2}^{n+1}+b_3u_{j3}^{n+1}+b_4u_{j4}^{n+1}+b_6 \tag{3.124}$$

$$v_2^* = b_1v_{j1}^{n+1}+b_2v_{j2}^{n+1}+b_3v_{j3}^{n+1}+b_4v_{j4}^{n+1}+b_7 \tag{3.125}$$

$$H_3^* = d_1H_{m1}^{n+1}+d_2H_{m2}^{n+1}+d_3H_{m3}^{n+1}+d_4H_{m4}^{n+1}+d_5 \tag{3.126}$$

$$u_3^* = d_1u_{m1}^{n+1}+d_2u_{m2}^{n+1}+d_3u_{m3}^{n+1}+d_4u_{m4}^{n+1}+d_6 \tag{3.127}$$

$$v_3^* = d_1v_{m1}^{n+1}+d_2v_{m2}^{n+1}+d_3v_{m3}^{n+1}+d_4v_{m4}^{n+1}+d_7 \tag{3.128}$$

in which k1, k2, k3, and k4 are nodes of the element that the backward tracking, along the first characteristic, stops in; j1, j2, j3, and j4 are nodes of the element that the backward tracking, along the second characteristic, stops in; m1, m2, m3, and m4 are nodes of the element that the backward tracking, along the third characteristic, stops in. (see the following figure)

Note: 1. $a_1 \sim a_4$, $b_1 \sim b_4$, and $d_1 \sim d_4$ are within the range of [0,1].
2. We may use two given parameters to determine where to stop in the backward tracking: one is for controlling tracking time and the other one is for controlling tracking distance.

Backward tracking along characteristics for 2-D overland flow

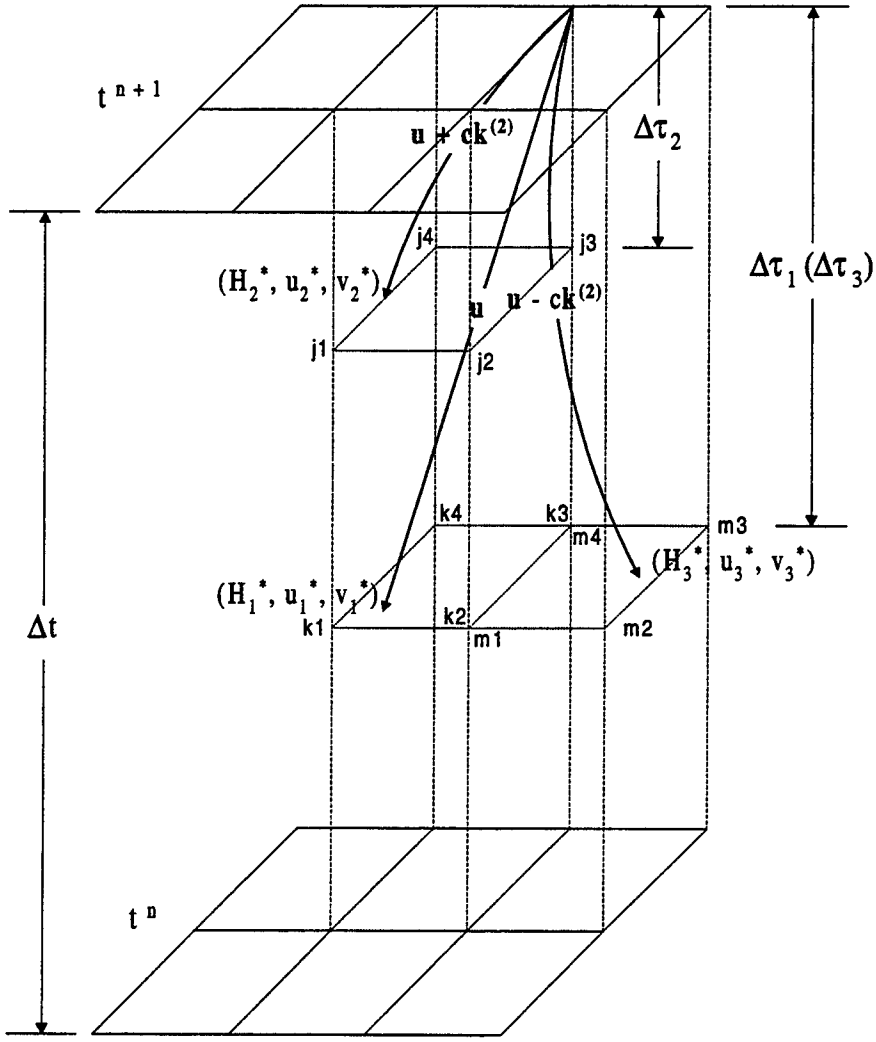

Figure 3.2. Tracking along characteristics in solving 2-D dynamic wave equation.

Eqs. (3.118) through (3.120) can be further expressed as

$$\frac{k_y^{(1)}}{\Delta\tau_1}\left(u-u_1^*\right)-\frac{k_x^{(1)}}{\Delta\tau_1}\left(v-v_1^*\right)+\frac{k_y^{(1)}}{h}(h\kappa+SS+R-I)u-\frac{k_x^{(1)}}{h}(h\kappa+SS+R-I)v$$

$$=-g\left(k_y^{(1)}\frac{\partial H}{\partial x}-k_x^{(1)}\frac{\partial H}{\partial y}\right)+k_y^{(1)}\frac{u^rR-u^iI}{h}-k_x^{(1)}\frac{v^rR-v^iI}{h}+k_y^{(1)}\frac{\tau_x^s}{h\rho}-k_x^{(1)}\frac{\tau_y^s}{h\rho} \qquad (3.129)$$

$$\frac{1}{c\Delta\tau_2}\left(H-H_2^*\right)+\frac{k_x^{(2)}}{g\Delta\tau_2}\left(u-u_2^*\right)+\frac{k_y^{(2)}}{g\Delta\tau_2}\left(v-v_2^*\right)$$

$$+\frac{k_x^{(2)}}{gh}(h\kappa+SS+R-I)u+\frac{k_y^{(2)}}{gh}(h\kappa+SS+R-I)v-\frac{u}{c}\frac{\partial Z_0}{\partial x}-\frac{v}{c}\frac{\partial Z_0}{\partial y}$$

$$=\frac{1}{c}(SS+R-I)+\frac{k_x^{(2)}}{g}\frac{u^rR-u^iI}{h}+\frac{k_y^{(2)}}{g}\frac{v^rR-v^iI}{h} \tag{3.130}$$

$$+\frac{k_x^{(2)}}{g}\frac{\tau_x^s}{h\rho}+\frac{k_y^{(2)}}{g}\frac{\tau_y^s}{h\rho}-\frac{h}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x}+k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y}-k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]$$

$$\frac{-1}{c\Delta\tau_3}\left(H-H_3^*\right)+\frac{k_x^{(2)}}{g\Delta\tau_3}\left(u-u_3^*\right)+\frac{k_y^{(2)}}{g\Delta\tau_3}\left(v-v_3^*\right)$$

$$+\frac{k_x^{(2)}}{gh}(h\kappa+SS+R-I)u+\frac{k_y^{(2)}}{gh}(h\kappa+SS+R-I)v+\frac{u}{c}\frac{\partial Z_0}{\partial x}+\frac{v}{c}\frac{\partial Z_0}{\partial y}$$

$$=-\frac{1}{c}(SS+R-I)+\frac{k_x^{(2)}}{g}\frac{u^rR-u^iI}{h}+\frac{k_y^{(2)}}{g}\frac{v^rR-v^iI}{h} \tag{3.131}$$

$$+\frac{k_x^{(2)}}{g}\frac{\tau_x^s}{h\rho}+\frac{k_y^{(2)}}{g}\frac{\tau_y^s}{h\rho}+\frac{h}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x}+k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y}-k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right)\right]$$

In obtaining Eqs. (3.129) through (3.131), the following relationships have been employed.

$$\frac{\tau_x^b}{h\rho}=\kappa u \tag{3.132}$$

$$\frac{\tau_y^b}{h\rho}=\kappa v \tag{3.133}$$

$$F_{xx}=h\epsilon_{xx}\frac{\partial u}{\partial x} \tag{3.134}$$

$$F_{yy}=h\epsilon_{yy}\frac{\partial v}{\partial y} \tag{3.135}$$

$$F_{xy}=F_{yx}=h\epsilon_{xy}\left[\frac{\partial u}{\partial y}+\frac{\partial v}{\partial x}\right] \tag{3.136}$$

When u_1^*, v_1^*, H_2^*, u_2^*, v_2^*, H_3^*, u_3^*, and v_3^* are determined explicitly by using the spatial reach

out option in backward tracking (i.e., track backward all the way to the previous time), Eqs. (3.129) through (3.131) can be solved node by node ($H^{\#}$, $u^{\#}$, $v^{\#}$) as shown below.

Eqs. (3.129) through (3.131), after being multiplied by water depth (i.e., h), can be written as

$$a_{12}u + a_{13}v = b_1 \tag{3.137}$$

$$a_{21}H + a_{22}u + a_{23}v = b_2 \tag{3.138}$$

$$a_{31}H + a_{32}u + a_{33}v = b_3 \tag{3.139}$$

where

$$a_{12} = k_y^{(1)}\left[\frac{h}{\Delta\tau_1} + h\kappa + SS + R - I\right] \tag{3.140}$$

$$a_{13} = -k_x^{(1)}\left[\frac{h}{\Delta\tau_1} + h\kappa + R - I\right] \tag{3.141}$$

$$b_1 = \frac{hk_y^{(1)}}{\Delta\tau_1}u_1^* - \frac{hk_x^{(1)}}{\Delta\tau_1}v_1^* - gh\left(k_y^{(1)}\frac{\partial H}{\partial x} - k_x^{(1)}\frac{\partial H}{\partial y}\right) + k_y^{(1)}(u\,{}^rR - u\,{}^iI) - k_x^{(1)}(v\,{}^rR - v\,{}^iI) + k_y^{(1)}\frac{\tau_x^s}{\rho} - k_x^{(1)}\frac{\tau_y^s}{\rho} \tag{3.142}$$

$$a_{21} = \frac{h}{c\Delta\tau_2} \tag{3.143}$$

$$a_{22} = k_x^{(2)}\left[\frac{h}{g\Delta\tau_2} + \frac{1}{g}(h\kappa + SS + R - I)\right] - \frac{h}{c}\frac{\partial Z_0}{\partial x} \tag{3.144}$$

$$a_{23} = k_y^{(2)}\left[\frac{h}{g\Delta\tau_2} + \frac{1}{g}(h\kappa + SS + R - I)\right] - \frac{h}{c}\frac{\partial Z_0}{\partial y} \tag{3.145}$$

$$b_2 = \frac{h}{c\Delta\tau_2}H_2^* + \frac{hk_x^{(2)}}{g\Delta\tau_2}u_2^* + \frac{hk_y^{(2)}}{g\Delta\tau_2}v_2^* + \frac{h}{c}(SS + R - I) + \frac{k_x^{(2)}}{g}(u\,{}^rR - u\,{}^iI) + \frac{k_y^{(2)}}{g}(v\,{}^rR - v\,{}^iI) + \frac{k_x^{(2)}}{g}\frac{\tau_x^s}{\rho} + \frac{k_y^{(2)}}{g}\frac{\tau_y^s}{\rho} - \frac{h^2}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x} + k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y} - k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right] \tag{3.146}$$

$$a_{31} = \frac{-h}{c\Delta\tau_3} \tag{3.147}$$

$$a_{32} = k_x^{(2)}\left[\frac{h}{g\Delta\tau_3} + \frac{1}{g}(h\kappa + SS + R - I)\right] + \frac{h}{c}\frac{\partial Z_0}{\partial x} \tag{3.148}$$

$$a_{33} = k_y^{(2)}\left[\frac{h}{g\Delta\tau_3} + \frac{1}{g}(h\kappa + SS + R - I)\right] + \frac{h}{c}\frac{\partial Z_0}{\partial y} \tag{3.149}$$

$$b_3 = \frac{-h}{c\Delta\tau_3}H_3^* + \frac{hk_x^{(2)}}{g\Delta\tau_3}u_3^* + \frac{hk_y^{(2)}}{g\Delta\tau_3}v_3^* - \frac{h}{c}(SS + R - I) + \frac{k_x^{(2)}}{g}(u^r R - u^i I) + \frac{k_y^{(2)}}{g}(v^r R - v^i I)$$
$$+ \frac{k_x^{(2)}}{g}\frac{\tau_x^s}{\rho} + \frac{k_y^{(2)}}{g}\frac{\tau_y^s}{\rho} + \frac{h^2}{c}\left[k_y^{(2)}k_y^{(2)}\frac{\partial u}{\partial x} + k_x^{(2)}k_x^{(2)}\frac{\partial v}{\partial y} - k_x^{(2)}k_y^{(2)}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right] \tag{3.150}$$

Therefore, we solve Eqs. (3.137) through (3.139) for $H^{\#}$, $u^{\#}$, $v^{\#}$ arithmetically. Now, we can solve Eq. (3.94) as follows. Eq. (3.94) can be written in details as

$$\frac{H - H^{\#}}{\Delta t} = 0 \tag{3.151}$$

$$\frac{h(u - u^{\#})}{\Delta t} = \left[\frac{\partial F_{xx}}{\partial x} + \frac{\partial F_{yx}}{\partial y}\right] \tag{3.152}$$

$$\frac{h(v - v^{\#})}{\Delta t} = \left[\frac{\partial F_{xy}}{\partial x} + \frac{\partial F_{yy}}{\partial y}\right] \tag{3.153}$$

Eq. (3.151) gives that $H = H^{\#}$, while Eqs. (3.152) and (3.153) can be discretized, in the finite element method, as

$$\frac{h}{\Delta t}[QA]\{u\} + [QD^1]\{u\} + [QD^4]\{v\} = \{QR^1\} + \{BQ^1\} \tag{3.154}$$

$$\frac{h}{\Delta t}[QA]\{v\} + [QD^2]\{u\} + [QD^3]\{v\} = \{QR^2\} + \{BQ^2\} \tag{3.155}$$

where

$$QA_{i,j} = \sum_{e\in M_e}\int_{R_e} N_\alpha^e N_\beta^e \, dR \tag{3.156}$$

$$QD_{i,j}^1 = \sum_{e\in M_e}\int_{R_e} \nabla N_\alpha^e \cdot \begin{bmatrix} h\epsilon_{xx} & 0 \\ 0 & h\epsilon_{xy} \end{bmatrix} \cdot \nabla N_\beta^e \, dR \tag{3.157}$$

$$QD_{i,j}^{2} = \sum_{e\in M_e} \int_{R_e} \nabla N_\alpha^e \cdot \begin{bmatrix} 0 & h\epsilon_{xy} \\ 0 & 0 \end{bmatrix} \cdot \nabla N_\beta^e \, dR \tag{3.158}$$

$$QD_{i,j}^{3} = \sum_{e\in M_e} \int_{R_e} \nabla N_\alpha^e \cdot \begin{bmatrix} h\epsilon_{xy} & 0 \\ 0 & h\epsilon_{yy} \end{bmatrix} \cdot \nabla N_\beta^e \, dR \tag{3.159}$$

$$QD_{i,j}^{4} = \sum_{e\in M_e} \int_{R_e} \nabla N_\alpha^e \cdot \begin{bmatrix} 0 & 0 \\ h\epsilon_{xy} & 0 \end{bmatrix} \cdot \nabla N_\beta^e \, dR \tag{3.160}$$

$$QR_i^1 = \sum_{e\in M_e} \int_{R_e} N_\alpha^e \frac{hu^\#}{\Delta t} \, dR \tag{3.161}$$

$$QR_i^2 = \sum_{e\in M_e} \int_{R_e} N_\alpha^e \frac{hv^\#}{\Delta t} \, dR \tag{3.162}$$

$$BQ_i^1 = \sum_{e\in M_e} \int_{B_e} \left\{ N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} h\epsilon_{xx} & 0 \\ 0 & h\epsilon_{xy} \end{bmatrix} \cdot \nabla u + N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} 0 & 0 \\ h\epsilon_{xy} & 0 \end{bmatrix} \cdot \nabla v \right\} dB \tag{3.163}$$

$$BQ_i^2 = \sum_{e\in M_e} \int_{B_e} \left\{ N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} 0 & h\epsilon_{xy} \\ 0 & 0 \end{bmatrix} \cdot \nabla u + N_\alpha^e \mathbf{n} \cdot \begin{bmatrix} h\epsilon_{xy} & 0 \\ 0 & h\epsilon_{yy} \end{bmatrix} \cdot \nabla v \right\} dB \tag{3.164}$$

In solving Eqs. (3.129) through (3.131) at boundary nodes, we demonstrate how boundary conditions are implemented as in the following. An overland boundary segment can be either an closed or an open (flow-through) boundary. In the former case, nothing needs to specify. While in the latter case, H, u, and v of the approaching flow, with respect to the characteristic ongoing direction, must be given at all segments (or segment nodes). Some details are given for both cases.

< Case 1> Closed boundaries: The first characteristic equation is always replaced by the following equation, representing a zero normal flux on the boundary.

$$\mathbf{n} \cdot \mathbf{u} = 0 \tag{3.165}$$

where **n** is the outward unit normal vector of the boundary segment. Tracking along the closed boundary will be used for the second and third characteristics if necessary.

< Case 2 > Open boundaries: The first characteristic equation is always replaced by the following equation, representing a zero lateral flux on the boundary.

$$\mathbf{n}_\perp \cdot \mathbf{u} = 0 \tag{3.166}$$

where $\mathbf{n}_\perp$ is the unit vector parallel to the segment. Either the second or the third characteristic equation, depending on the propagation direction, will be replaced by the boundary condition specified on the boundary. There are four types of boundary conditions considered here. Only when the propagation direction is inward to the domain of interest, will the replacement be employed.

(1) Given time-dependent normal flux, q(t): (used for upstream open boundaries)

$$\mathbf{n}\cdot\mathbf{u} = \frac{q}{h} \tag{3.167}$$

(2) Given time-dependent water stage, H(t): (used for either upstream or downstream boundaries)

$$H = H_b \tag{3.168}$$

(3) Given water depth-dependent normal flux, q(h): (used for natural downstream open boundaries or river/stream-/junction-related boundaries)

$$\mathbf{n}\cdot\mathbf{u} = \frac{q}{h} \tag{3.169}$$

(4) Given stage difference-dependent normal flux, q(ΔH): (used for river/stream-/junction-related boundaries)

$$\mathbf{n}\cdot\mathbf{u} = \frac{q_n}{h} \tag{3.170}$$

As mentioned earlier in Section 3.1.2, both depth and velocity must be specified on the boundary where super-critical flow occurs.

3.2.2. The Lagrangian approach for both 2-D diffusion and 2-D kinematic wave models

Recall Eqs. (2.9), (2.12), and (2.13)

$$\frac{\partial h}{\partial t} + \frac{\partial hu}{\partial x} + \frac{\partial hv}{\partial y} = SS + R - I \tag{3.171}$$

where

$$u = \frac{-1}{n}\left[\frac{h}{1+(\nabla Z_0)^2}\right]^{2/3} \frac{1}{[\nabla(Z_0+h)]^{1/2}} \frac{\partial(Z_0+h)}{\partial x} \tag{3.172}$$

$$v = \frac{-1}{n}\left[\frac{h}{1+(\nabla Z_0)^2}\right]^{2/3} \frac{1}{[\nabla(Z_0+h)]^{1/2}} \frac{\partial(Z_0+h)}{\partial y} \tag{3.173}$$

Substituting Eqs. (3.168) and (3.169) into Eq. (3.167) yields

$$\frac{\partial h}{\partial t} + \frac{5u}{3}\frac{\partial h}{\partial x} + \frac{5v}{3}\frac{\partial h}{\partial y} = SS + R - I - X - Y \tag{3.174}$$

where

$$X = \frac{-1}{n}\frac{h^{5/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{1}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial^2(Z_0+h)}{\partial x^2}+\frac{1}{n^2}\frac{h^{5/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{1}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial(Z_0+h)}{\partial x}\frac{\partial n}{\partial x}$$

$$+\frac{-2}{n}\frac{h^{5/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{\partial(Z_0+h)}{\partial x}\frac{-1}{4}\left[\left(\frac{\partial(Z_0+h)}{\partial x}\right)^2+\left(\frac{(Z_0+h)}{\partial y}\right)^2\right]^{-5/4} \tag{3.175}$$

$$\left[\frac{\partial(Z_0+h)}{\partial x}\frac{\partial^2(Z_0+h)}{\partial x^2}+\frac{\partial(Z_0+h)}{\partial y}\frac{\partial^2(Z_0+h)}{\partial x\partial y}\right]$$

$$+\frac{-2}{n}\frac{h^{5/3}}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial(Z_0+h)}{\partial x}\frac{-2}{3}\left[1+(\nabla Z_0)^2\right]^{-5/3}\left[\frac{\partial Z_0}{\partial x}\frac{\partial^2 Z_0}{\partial x^2}+\frac{\partial Z_0}{\partial y}\frac{\partial^2 Z_0}{\partial x\partial y}\right]$$

$$Y = \frac{-1}{n}\frac{h^{5/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{1}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial^2(Z_0+h)}{\partial y^2}+\frac{1}{n^2}\frac{h^{5/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{1}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial(Z_0+h)}{\partial y}\frac{\partial n}{\partial y}$$

$$+\frac{-2}{n}\frac{h^{5/3}}{\left[1+(\nabla Z_0)^2\right]^{2/3}}\frac{\partial(Z_0+h)}{\partial y}\frac{-1}{4}\left[\left(\frac{\partial(Z_0+h)}{\partial x}\right)^2+\left(\frac{(Z_0+h)}{\partial y}\right)^2\right]^{-5/4} \tag{3.176}$$

$$\left[\frac{\partial(Z_0+h)}{\partial x}\frac{\partial^2(Z_0+h)}{\partial x\partial y}+\frac{\partial(Z_0+h)}{\partial y}\frac{\partial^2(Z_0+h)}{\partial y^2}\right]$$

$$+\frac{-2}{n}\frac{h^{5/3}}{[\nabla(Z_0+h)]^{1/2}}\frac{\partial(Z_0+h)}{\partial y}\frac{-2}{3}\left[1+(\nabla Z_0)^2\right]^{-5/3}\left[\frac{\partial Z_0}{\partial x}\frac{\partial^2 Z_0}{\partial x\partial y}+\frac{\partial Z_0}{\partial y}\frac{\partial^2 Z_0}{\partial y^2}\right]$$

Eq. (3.174) can be further written as

$$\frac{Dh}{Dt} = SS+R-I-X-Y \tag{3.177}$$

where the following characteristic equations apply.

$$\frac{dx}{dt} = \frac{5}{3}u \tag{3.178}$$

$$\frac{dy}{dt} = \frac{5}{3}v \tag{3.179}$$

Hence the solution to Eq. (3.177) is

$$h(x,y,t) = h(x_0,y_0,0)+(R-I-X-Y)t \tag{3.180}$$

in which

$$x - x_0 = \int_0^t \frac{5}{3} u dt \tag{3.181}$$

$$y - y_0 = \int_0^t \frac{5}{3} v dt \tag{3.182}$$

A nonlinear iteration loop with the Picard method implemented is used to solve Eqs. (3.78) through (3.80) in the dynamic wave model or to solve Eqs. (3.171) through (3.173) in the diffusion wave model during each time step.

3.3. Solving the 1-D river/stream transport equations

In solving the transport equations of both 1-D river/stream and 2-D overland, the following strategy is employed.

<Stategy> Using the predictor-corrector scheme to deal with transport equations of mobile materials.

In solving Eqs. (2.23), (2.25), and (2.26), the following strategy is employed. All the three equations can be expressed in the following form.

$$A\frac{dC}{dt} = L(C) + RHS \tag{3.183}$$

where C can be S_n, C_i^w, or $S_n C_{ni}^s$, L is the diffusion operator, and RHS represents source/sink terms. Thus, we can solve Eq. (3.183) with the following two steps.

First, we solve

$$A\frac{C^{N+1/2} - C^N}{\Delta\tau} = L(C^{N+1/2}) + (RHS)^N \tag{3.184}$$

Second, we solve

$$A\frac{C^{N+1} - C^N}{\Delta\tau} = L(C^{N+1/2}) + (RHS)^{N+1} \tag{3.185}$$

We can also subtract Eq. (3.185) by Eq. (3.184) to yield

$$A\frac{C^{N+1} - C^{N+1/2}}{\Delta\tau} = (RHS)^{N+1} - (RHS)^N \tag{3.186}$$

The advantage of solving Eq. (3.186), rather than Eq. (3.185), is that we can compute C^{N+1} node by node when $C^{N+1/2}$ is previously determined. Thus, we first solve Eq. (3.184) for $C^{N+1/2}$ (the intermediate value) in the so-called predictor step and perform the so-called corrector step by solving Eq. (3.186) to obtain C^{N+1}. To avoid negative numerical results in solving Eq. (3.184), the following

equation is actually solved when $(RHS)^N$ is negative.

$$A\frac{C^{N+1/2}-C^N}{\Delta\tau}-\frac{(RHS)^N}{C^N}C^{N+1/2} = L(C^{N+1/2}) \tag{3.187}$$

Consequently, we are solving the following equation in the corrector step.

$$A\frac{C^{N+1}-C^{N+1/2}}{\Delta\tau} = (RHS)^{N+1}-\frac{(RHS)^N}{C^N}C^{N+1/2} \tag{3.188}$$

With the finite element approximation, Eq. (3.184) can be discretized as follows.

$$\left(\frac{[QA]}{\Delta\tau}+w[QD]\right)\{C\} = \{QR\}+(1-w)[QD]\{C^p\}+\{QB\} \tag{3.189}$$

where the associated element matrices are defined as follows.

$$[QA]^e = \int_e N_i A N_j dx \tag{3.190}$$

$$[QD]^e = \int_e \frac{dN_i}{dx} A K_x \frac{dN_j}{dx} dx \tag{3.191}$$

$$\{QR\}^e = \int_e N_i (RHS)^N dx \tag{3.192}$$

$$\{QB\}^e = -\left(-AK_x\frac{\partial C}{\partial x}\right)_{boundary} \tag{3.193}$$

It is noted that both $[QA]^e$ and $\{QR\}^e$ must be lumped such that Eqs. (3.184) and (3.186) are solved consistently. Also, boundary conditions for mobile materials are implemented in this predictor step.

In the following, we are to show the procedures of solving the transport system in Section 3.3.1, to determine the concentrations of contaminants and sediments at junctions in Section 3.3.2, and to give estimation of deposition and erosion in Section 3.3.3.

3.3.1. Procedures of solving 1-D river/stream transport equations

Recall Eqs. (2.23) through (2.27) and express them in the Lagrangian form for mobile materials as follows.

For the continuity equation of suspended sediment:

$$A\frac{dS_n}{dt} = A\frac{\partial S_n}{\partial t}+Q\frac{\partial S_n}{\partial x} = 0 \tag{3.194}$$

$$A\frac{dS_n}{dt}-\frac{\partial}{\partial x}\left[AK_x\frac{\partial S_n}{\partial x}\right]=\left[M_n^s+PR_n-PD_n+M_n^{os}\right]-\left[SS+R-I+R_1+R_2\right]S_n \qquad n\in[1,N_s] \quad (3.195)$$

For the continuity equation of bed sediment:

$$\frac{\partial M_n}{\partial t}=D_n-R_n \qquad n\in[1,N_s] \quad (3.196)$$

For the continuity equation of dissolved chemical:

$$A\frac{dC_i^w}{dt}=A\frac{\partial C_i^w}{\partial t}+Q\frac{\partial C_i^w}{\partial x}=0 \quad (3.197)$$

$$\begin{aligned}A\frac{dC_i^w}{dt}-\frac{\partial}{\partial x}\left[AK_x\frac{\partial C_i^w}{\partial x}\right]=&\\ &\left[M_i^{cw}+Ak_i^{ab}p_i+\sum_{n=1}^{N_s}k_{ni}^{sb}S_nAC_{ni}^s+\sum_{n=1}^{N_s}k_{ni}^{bb}M_nPC_{ni}^b+M_i^{crw}-M_i^{ciw}+M_i^{cow}\right]\\ &+\sum_{m=1}^{N_{rx}}(a_{mj}-b_{mj})k_m^{rb}A\left[\prod_{j=1}^{N_c}(C_j^w)^{b_{mj}}-\frac{k_m^{rf}}{k_m^{rb}}\prod_{j=1}^{N_c}(C_j^w)^{a_{mj}}\right]\\ &-\left[\lambda_i^wA+Ak_i^{af}+\sum_{n=1}^{N_s}S_nAk_{ni}^{sf}+\sum_{n=1}^{N_s}M_nPk_{ni}^{bf}+SS+R-I+R_1+R_2\right]C_i^w \qquad i\in[1,N_c]\end{aligned} \quad (3.198)$$

For the continuity equation of particulate chemical on suspended sediment:

$$A\frac{d(S_nC_{ni}^s)}{dt}=A\frac{\partial(S_nC_{ni}^s)}{\partial t}+Q\frac{\partial(S_nC_{ni}^s)}{\partial x}=0 \quad (3.199)$$

For the continuity equation of particulate chemical on bed sediment:

$$\frac{\partial(M_nC_{ni}^b)}{\partial t}=\left[D_nC_{ni}^s-R_nC_{ni}^b+k_{ni}^{bf}M_nC_i^w\right]-\left[\lambda_{ni}^b+k_{ni}^{bb}\right]M_nC_{ni}^b \qquad n\in[1,N_s],i\in[1,N_c] \quad (3.200)$$

We solve the transport system by achieving the following steps.

Step 1 Solve Eqs. (3.194), (3.197), and (3.199) to obtain the Lagrangian values for suspended sediments, dissolved chemicals, and particulate chemicals on suspend sediments.

Step 2 Solve Eqs. (3.195) and (3.196) for S_n and M_n.

(a) Solve Eq. (3.195) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eq. (3.195)) and obtain *the intermediate value* for suspended sediments.

(b) Prepare the corrector form of Eqs. (3.195) as described in Eq. (3.186). It can be written as follows.

$$A\frac{(S_n)^{N+1}-(S_n)^{N+1/2}}{\delta t}$$

$$= (RHS_n^s)^{N+1}-(RHS_n^s)^N \quad \left(\text{if } (RHS_n^s)^N \geq 0\right) \tag{3.201}$$

$$= (RHS_n^s)^{N+1}-\frac{(RHS_n^s)^N}{(S_n)^N}(S_n)^{N+1/2} \left(\text{if } (RHS_n^s)^N<0\right) \qquad n\in[1,N_s]$$

where

$$(RHS_n^s) = \left[M_n^s+PR_n-PD_n+M_n^{os}\right]+\left[SS+R-I+R_1+R_2\right]S_n \qquad n\in[1,N_s] \tag{3.202}$$

(c) Solve Eq. (3.202) and Eq. (3.196) node by node with the Picard method to obtain the concentrations of suspended and bed sediments.

Note: In Eqs. (3.195) and (3.196) both D_n and R_n need to be evaluated first, while in Eq. (3.195) A, Q, K_x, P, R, I, R_1, R_2, M_t^s, and M_t^{os} are either given or determined after the flow equations are solved. During each iteration in (c), both Eq. (3.202) and (3.196) are solved with the time-implicit scheme.

Step 3 Solve Eqs. (3.198), (3.200), and (3.201) for C_i^w, C_{ni}^s, and C_{ni}^b.

(a) Solve Eqs. (3.198) and (3.200) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eqs. (3.198) and (3.200)).
(b) Prepare the corrector form of Eqs. (3.198) and (3.200) described in Eq. (3.186). They can be written as follows.

For dissolved chemicals:

$$A\frac{(C_i^w)^{N+1}-(C_i^w)^{N+1/2}}{\delta t}$$

$$= (RHS_i^w)^{N+1}-(RHS_i^w)^N \quad \left(\text{if } (RHS_i^w)^N \geq 0\right) \tag{3.203}$$

$$= (RHS_i^w)^{N+1}-\frac{(RHS_i^w)^N}{(C_i^w)^N}(C_i^w)^{N+1/2} \left(\text{if } (RHS_i^w)^N<0\right) \qquad i\in[1,N_c]$$

where

$$
\begin{aligned}
(RHS_i^w) &= \left[M_i^{cw} + Ak_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n A C_{ni}^s + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n P C_{ni}^b + M_i^{crw} - M_i^{ciw} + M_i^{cow}\right] \\
&\quad - \left[\lambda_i^w A + Ak_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} + SS + R - I + R_1 + R_2\right] C_i^w \\
&\quad + \sum_{m=1}^{N_{rx}} (a_{mj} - b_{mj}) k_m^{rb} A \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}}\right] \qquad i \in [1, N_c]
\end{aligned} \tag{3.204}
$$

For particulate chemicals on suspended sediments:

$$
\begin{aligned}
&A \frac{(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}}{\delta t} \\
&= (RHS_{ni}^s)^{N+1} - (RHS_{ni}^s)^N \quad \left(\text{if } (RHS_{ni}^s)^N \geq 0\right) \\
&= (RHS_{ni}^s)^{N+1} - \frac{(RHS_{ni}^s)^N}{(C_{ni}^s)^N} (C_{ni}^s)^{N+1/2} \quad \left(\text{if } (RHS_{ni}^s)^N < 0\right) \qquad n \in [1, N_s],\ i \in [1, N_c]
\end{aligned} \tag{3.205}
$$

where

$$
\begin{aligned}
(RHS_{ni}^s) &= \left[M_{ni}^{cs} + k_{ni}^{sf} S_n A C_i^w + BR_n C_{ni}^b - BD_n C_{ni}^s + M_{ni}^{cos}\right] \\
&\quad - \left[\lambda_{ni}^s A + k_{ni}^{sb} A + SS + R - I + R_1 + R_2\right] S_n C_{ni}^s \qquad n \in [1, N_s],\ i \in [1, N_c]
\end{aligned} \tag{3.206}
$$

(c) Solve Eqs. (3.204), (3.206), and (3.201) node by node with the Newton-Raphson method.

Note: In Eqs. (3.204), (3.206), and (3.201) S_n and M_n are computed in Step 1, while A, Q, B, P, K_x, reaction rate constants, stoichiometry, 1-st order decay constants, partial atmospheric pressure, and sources/sinks are either given or determined after the flow equations are solved.

To achieve the (c) of Step 3, the following residual equations are constructed.

For dissolved chemicals:

$$
\begin{aligned}
&(RES_i^w) \\
&= A\left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2}\right] - \delta t \left[(RHS_i^w)^{N+1} - (RHS_i^w)^N\right] \quad \left(\text{if } (RHS_i^w)^N \geq 0\right) \\
&= A\left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2}\right] - \delta t \left[(RHS_i^w)^{N+1} - \frac{(RHS_i^w)^N}{(C_i^w)^N} (C_i^w)^{N+1/2}\right] \quad \left(\text{if } (RHS_i^w)^N < 0\right) \\
&\qquad\qquad i \in [1, N_c]
\end{aligned} \tag{3.207}
$$

For particulate chemicals on suspended sediments:

$$(RES_{ni}^{s})$$

$$= A\left[(S_n C_{ni}^{s})^{N+1} - (S_n C_{ni}^{s})^{N+1/2}\right] - \delta t\left[(RHS_{ni}^{s})^{N+1} - (RHS_{ni}^{s})^{N}\right] \quad \left(\text{if } (RHS_{ni}^{s})^{N} \geq 0\right)$$

$$= A\left[(S_n C_{ni}^{s})^{N+1} - (S_n C_{ni}^{s})^{N+1/2}\right] - \delta t\left[(RHS_{ni}^{s})^{N+1} - \frac{(RHS_{ni}^{s})^{N}}{(C_{ni}^{s})^{N}}(C_{ni}^{s})^{N+1/2}\right] \quad \left(\text{if } (RHS_{ni}^{s})^{N} < 0\right) \tag{3.208}$$

$$n \in [1,N_s], \quad i \in [1,N_c]$$

For particulate chemicals on bed sediments:

$$(RES_{ni}^{b}) = (M_n C_{ni}^{b})^{N+1} - (M_n C_{ni}^{b})^{N} - \Delta t\,(RHS_{ni}^{b})^{N+1} \qquad n \in [1,N_s], \quad i \in [1,N_c] \tag{3.209}$$

The associated Jacobian entries are thus computed as shown in the following.

For dissolved chemicals:

$$\frac{\partial(RES_i^{w})}{\partial(C_l^{w})^{N+1}} = \delta_{il} A + \delta_{il}\,\delta t\left[\lambda_i^{w} A + SS + R - I + R_1 + R_2 + A k_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf}\right] -$$

$$\delta t\left[\sum_{m=1}^{N_{rx}} (a_{mi} - b_{mi}) A\left(k_m^{rb} b_{ml} (C_l^{w})^{b_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{w})^{b_{mj}} - k_m^{rf} a_{ml} (C_l^{w})^{a_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{w})^{a_{mj}}\right)\right] \tag{3.210}$$

$$i \in [1,N_c]$$

$$\frac{\partial(RES_i^{w})}{\partial(C_{nl}^{s})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sb} S_n A \qquad n \in [1,N_s], \quad i \in [1,N_c], \tag{3.211}$$

$$\frac{\partial(RES_i^{w})}{\partial(C_{nl}^{b})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{bb} M_n P \qquad n \in [1,N_s], \quad i \in [1,N_c] \tag{3.212}$$

For particulate chemicals on suspended sediments:

$$\frac{\partial(RES_{ni}^{s})}{\partial(C_l^{w})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sf} S_n A \qquad n \in [1,N_s], \quad i \in [1,N_c] \tag{3.213}$$

$$\frac{\partial(RES_{ni}^{s})}{\partial(C_{nl}^{s})^{N+1}} = \delta_{il} A S_n + \delta_{il}\,\delta t\, B D_n + \delta_{il}\,\delta t\, S_n\left[\lambda_{ni}^{s} A + k_{ni}^{sb} A + SS + R - I + R_1 + R_2\right] \tag{3.214}$$

$$n \in [1,N_s], \quad i \in [1,N_c]$$

$$\frac{\partial(RES_{ni}^{s})}{\partial(C_{nl}^{b})^{N+1}} = -\delta_{il}\,\delta t\,BR_n \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.215}$$

For particulate chemicals on bed sediments:

$$\frac{\partial(RES_{ni}^{b})}{\partial(C_{l}^{w})^{N+1}} = -\delta_{il}\,\Delta t\,k_{ni}^{bf}M_n \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.216}$$

$$\frac{\partial(RES_{ni}^{b})}{\partial(C_{nl}^{s})^{N+1}} = -\delta_{il}\,\Delta t\,D_n \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.217}$$

$$\frac{\partial(RES_{ni}^{b})}{\partial(C_{nl}^{b})^{N+1}} = \delta_{il}M_n + \delta_{il}\,\Delta t\,R_n + \delta_{il}\,\Delta t\,M_n\left[\lambda_{ni}^{b} + k_{ni}^{bb}\right] \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.218}$$

3.3.2. Determining contaminant and sediment concentrations at junctions

At junctions, the following equations are employed to determine the concentrations of contaminants and sediments.

For suspended sediment:

$$\frac{dV(j)S_n(j)}{dt} = \sum_{k=1}^{NJRTH(j)} Q^{k}S_n^{k} + M_n^{s}(j) + M_n^{os}(j) + [R_n(j) - D_n(j)]AJT(j) \qquad n\in[1,N_s] \tag{3.219}$$

For bed sediment:

$$\frac{\partial M_n(j)}{\partial t} = D_n(j) - R_n(j) \qquad n\in[1,N_s] \tag{3.220}$$

For dissolved chemical:

$$\frac{dV(j)C_i^w(j)}{dt}$$

$$= \sum_{k=1}^{NJRTH(j)} Q^k C_i^{wk} + M_i^{cw}(j) - \lambda_i^w V(j) C_i^w(j) + M_i^{crw}(j) - M_i^{ciw}(j) + M_i^{cow}(j)$$

$$+ V(j) k_i^{ab} \left[p_i - \frac{k_i^{af}}{k_i^{ab}} C_i^w(j) \right] + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n(j) V(j) \left[C_{ni}^s(j) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w(j) \right] \qquad (3.221)$$

$$+ \sum_{n=1}^{N_s} k_{ni}^{bb} M_n(j) AJT(j) \left[C_{ni}^b(j) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w(j) \right]$$

$$+ \sum_{m=1}^{N_{rx}} (a_{mi} - b_{mi}) k_m^{rb} V(j) \left[\prod_{j=1}^{N_c} \left(C_j^w(j) \right)^{b_{mj}} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} \left(C_j^w(j) \right)^{a_{mj}} \right] \qquad i \in [1, N_c]$$

For particulate chemical on suspended sediment:

$$\frac{dV(j)S_n(j)C_{ni}^s(j)}{dt}$$

$$= \sum_{k=1}^{NJRTH(j)} Q^k S_n C_{ni}^{sk} + M_{ni}^{cs}(j) - \lambda_{ni}^s V(j) S_n(j) C_{ni}^s(j) \qquad (3.222)$$

$$- k_{ni}^{sb} S_n(j) V(j) \left[C_{ni}^s(j) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w(j) \right] + R_n(j) AJT(j) C_{ni}^b(j) - D_n(j) AJT(j) C_{ni}^s(j) + M_{ni}^{cos}(j)$$

$$n \in [1, N_s],\ i \in [1, N_c]$$

For particulate chemical on bed sediment:

$$\frac{\partial [M_n(j) C_{ni}^b(j)]}{\partial t}$$

$$= [D_n(j) C_{ni}^s(j) - R_n(j) C_{ni}^b(j)) - \lambda_{ni}^b(j) M_n(j) C_{ni}^b(j) - k_{ni}^{bb} M_n(j) \left[C_{ni}^b(j) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w(j) \right] \qquad (3.223)$$

$$n \in [1, N_s], i \in [1, N_c]$$

where

$V(j)$ = The volume of water at the j-th junction [L^3];

$AJT(j)$ = The horizontal area of the j-th junction [L^2].

$D_n(j)$ = Deposition rate of the n-th size fraction sediment at the j-th junction [$M/L^2/T$];

$R_n(j)$ = Erosion rate of the n-th size fraction sediment [$M/L^2/T$];

$S_n(j)$ = Volumetrically averaged sediment concentration of the n-th fraction size at the j-th junction [M/L^3];

$M_n(j)$ = Sediment mass per unit bed area of the n-th size fraction at the j-th junction at the j-th junction [M/L^2];

NJRTH(j) =Number of river/stream reaches which connect to the j-th junction;

Q^k = The flow rate from the k-th connected river/stream reach to the junction [L^3/T], it is positive if coming in and negative if going out;

S_n^k = The concentration of the n-th sized suspended sediment from the k-th connected river/stream reach to the junction [M/L^3];

C_i^{wk} = The concentration of the i-th dissolved chemical from the k-th connected river/stream reach to the junction [M/L^3];

C_{ni}^{sk} = The concentration of the i-th particulate chemical on the n-th sized suspended sediment from the k-th connected river/stream reach to the junction [M/L^3];

$M_n^s(j)$ = Source of the n-th suspended sediment at the j-th junction [M/T];

$M_n^{os}(j)$ = Source of the n-th suspended sediment from overland flow to the j-th junction [M/T];

$C_i^w(j)$ = Volometrically-averaged concentration of the i-th dissolved chemical at the j-th junction [M/L^3];

$C_{ni}^b(j)$ = Volometrically-averaged particulate chemical concentration on bed sediment of the n-th fraction size at the j-th junction [M/M];

$C_{ni}^s(j)$ = Volometrically-averaged particulate chemical concentration on suspended sediment of the n-th fraction size at the j-th junction [M/M];

$M_{ni}^{cs}(j)$ = Source of the i-th particulate chemical on suspended sediment of the n-th fraction size at the j-th junction [M/T];

$M_{ni}^{cos}(j)$ = Source of the i-th particulate chemical on suspended sediment of the n-th fraction size from overland to the j-th junction [M/T];

$M_i^{cw}(j)$ = Source of the i-th dissolved chemical at the j-th junction [M/T];

$M_i^{crw}(j)$ = Rainfall source of the i-th dissolved chemical at the j-th junction [M/T];

$M_i^{ciw}(j)$ = Infiltration sink of the i-th dissolved chemical at the j-th junction [M/T];

$M_i^{cow}(j)$ = Source of the i-th dissolved chemical from overland to the j-th junction [M/T].

Eqs. (3.220) and (3.221) are solved first by using the Picard method, while Eqs. (3.222) through (3.224) are solved with the Newton-Raphson method.

3.3.3. Estimation of Deposition and Erosion

We estimate the deposition and erosion rates by using the following equations.

< Case 1 > Cohesive sediments (e.g., silt and clay):

$$D_n = V_{sn} S_n \left[1 - \frac{\tau_b}{\tau_{cDn}} \right] \tag{3.224}$$

$$R_n = E_n\left[\frac{\tau_b}{\tau_{cRn}} - 1\right] \tag{3.225}$$

where V_{sn} is the settling velocity of the n-th size fraction sediment [L/T]; τ_b is the bottom shear stress or the bottom friction stress [M/L/T^2]; τ_{cDn} is the critical shear stress for the deposition of the n-th size fraction sediment [M/L/T^2]; τ_{cRn} is the critical shear stress for the erosion of the n-th size fraction sediment [M/L/T^2]; E_n is the erodibility of the n-th size fraction sediment [M/L^2]. In the computer code, V_{sn}, τ_{cDn}, τ_{cRn}, and E_n are input parameters, while τ_b is computed in the flow module.

< Case 2 > Non-cohesive sediments (e.g., sand):

$$D_n = \frac{G_{sAn} - G_{sn}}{\Delta L} \tag{3.226}$$

$$R_n = \frac{G_{sn} - G_{sAn}}{\Delta L} \tag{3.227}$$

where G_{sAn} is the actual load rate of the n-th size fraction sediment per unit width at a upstream location [M/L/T]; G_{sn} is the maximum load rate (capacity) of the n-th size fraction sediment per unit width at a downstream location [M/L/T]; ΔL is the distance between the upstream and the downstream locations. In the computer code, ΔL can be determined based on the coordinates, while G_{sAn} and G_{sn} are computed based on the following equations.

$$G_{sAn} = S_n * u * r \tag{3.228}$$

$$G_{sn} = 10\frac{\rho^2 u\, r\, S\,(\tau_b - \tau_{crn})}{g\, d_n\,(\rho_{sn} - \rho)^2} \tag{3.229}$$

where ρ is the fluid density [M/L^3]; ρ_{sn} is the density of the n-th size fraction sediment [M/L^3]; u is river/stream flow velocity [L/T]; r is hydraulic radius [L]; S the friction slope, d_n is the median diameter of the n-th size fraction sediment particle [L]; g is gravity [L/T^2]; τ_{crn} is the critical bottom shear stress of the n-th size fraction sediment at which sediment movement begins [M/L/T^2]. Among these parameters, ρ, ρ_{sn}, d_n, and τ_{crn} are input by users, while u, r, and S are estimated in the flow module.

3.4. Solving the 2-D overland transport equations

The strategy for solving 2-D overland transport equations has been described in the previous section and will not be repeated here. In the following, we are to go through the procedures of solving the 2-D transport system, like what we have achieved in Section 3.3.1 for 1-D river/stream transport. Recall Eqs. (2.41) through (2.45) and express them in the Lagrangian form for mobile materials as follows.

For the continuity equation of suspended sediment:

$$h\frac{dS_n}{dt} = h\frac{\partial S_n}{\partial t} + \mathbf{q}\cdot\nabla S_n = 0 \tag{3.230}$$

$$h\frac{dS_n}{dt} - \nabla\cdot\left[h\mathbf{K}\cdot\nabla S_n\right] = \left[M_n^s + R_n - D_n\right] - \left[SS + R - I\right]S_n \qquad n\in[1,N_s] \tag{3.231}$$

For the continuity equation of bed sediment:

$$\frac{\partial M_n}{\partial t} = D_n - R_n \qquad n\in[1,N_s] \tag{3.232}$$

For the continuity equation of dissolved chemical:

$$h\frac{dC_i^w}{dt} = h\frac{\partial C_i^w}{\partial t} + \mathbf{q}\cdot\nabla C_i^w = 0 \tag{3.233}$$

$$\begin{aligned} &h\frac{dC_i^w}{dt} - \nabla\cdot\left[h\mathbf{K}\cdot\nabla C_i^w\right] \\ &= \sum_{m=1}^{N_{rx}} (a_{mj} - b_{mj}) k_m^{rb} h \left[\prod_{j=1}^{N_c} (C_j^w)^{b_{mj}} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} (C_j^w)^{a_{mj}}\right] \\ &+ \left[M_i^{cw} + hk_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n h C_{ni}^s + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n C_{ni}^b + M_i^{crw} - M_i^{ciw}\right] \\ &- \left[\lambda_i^w h + hk_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} + SS + R - I\right] C_i^w \qquad i\in[1,N_c] \end{aligned} \tag{3.234}$$

For the continuity equation of particulate chemical on suspended sediment:

$$h\frac{d(S_n C_{ni}^s)}{dt} = h\frac{\partial(S_n C_{ni}^s)}{\partial t} + \mathbf{q}\cdot\nabla(S_n C_{ni}^s) = 0 \tag{3.235}$$

$$\begin{aligned} &h\frac{dS_n C_{ni}^s}{dt} - \nabla\cdot\left[h\mathbf{K}\cdot\nabla(S_n C_{ni}^s)\right] \\ &= \left[M_{ni}^{cs} + k_{ni}^{sf} h S_n C_i^w + R_n C_{ni}^b - D_n C_{ni}^s\right] - \left[\lambda_{ni}^s h + k_{ni}^{sb} h + SS + R - I\right] S_n C_{ni}^s \\ &\qquad\qquad n\in[1,N_s],\ i\in[1,N_c] \end{aligned} \tag{3.236}$$

For the continuity equation of particulate chemical on bed sediment:

$$\frac{\partial(M_n C_{ni}^b)}{\partial t} = \left[D_n C_{ni}^s - R_n C_{ni}^b + k_{ni}^{bf} M_n C_i^w\right] - \left[\lambda_{ni}^b + k_{ni}^{bb}\right] M_n C_{ni}^b \qquad n\in[1,N_s], i\in[1,N_c] \tag{3.237}$$

We solve the transport system by achieving the following steps.

Step 1 Solve Eqs. (3.231), (3.234), and (3.236) to obtain the Lagrangian values for suspended sediments, dissolved chemicals, and particulate chemicals on suspend sediments.

Step 2 Solve Eqs. (3.232) and (3.233) for S_n and M_n.

(a) Solve Eq. (3.232) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eq. (3.232)) and obtain *the intermediate value* for suspended sediments.
(b) Prepare the corrector form of Eqs. (3.232) as described in Eq. (3.186). It can be written as follows.

$$h\frac{(S_n)^{N+1}-(S_n)^{N+1/2}}{\delta t}$$

$$= (RHS_n^s)^{N+1}-(RHS_n^s)^N \quad \left(\text{if } (RHS_n^s)^N \geq 0\right) \tag{3.238}$$

$$= (RHS_n^s)^{N+1}-\frac{(RHS_n^s)^N}{(S_n)^N}(S_n)^{N+1/2} \left(\text{if } (RHS_n^s)^N<0\right) \qquad n\in[1,N_s]$$

where

$$(RHS_n^s) = \left[M_n^s+R_n-D_n\right]-[SS+R-I]S_n \qquad n\in[1,N_s] \tag{3.239}$$

(c) Solve Eq. (3.239) and Eq. (3.233) node by node with the Picard method to obtain the solutions for suspended and bed sediments.

*Note: In Eqs. (3.232) and (3.233) both D_n and R_n need to be evaluated first, while in Eq. (3.232) **K**, h, R, I, and SS are either given or determined after the flow equations are solved. During each iteration in (c), both Eq. (3.239) and (3.233) are solved with the time-implicit scheme.*

Step 3 Solve Eqs. (3.235), (3.237), and (3.238) for C_i^w, C_{ni}^s, and C_{ni}^b.

(a) Solve Eqs. (3.235) and (3.237) with all source/sink terms evaluated at the previous time, as described in Eq. (3.184). (the predictor process of Eqs. (3.235) and (3.237)).
(b) Prepare the corrector form of Eqs. (3.235) and (3.237) described in Eq. (3.186). They can be written as follows.

For dissolved chemicals:

$$h\frac{(C_i^{\,w})^{N+1}-(C_i^{\,w})^{N+1/2}}{\delta t}$$

$$= (RHS_i^{\,w})^{N+1}-(RHS_i^{\,w})^{N} \quad \left(\text{if } (RHS_i^{\,w})^{N}\geq 0\right) \tag{3.240}$$

$$= (RHS_i^{\,w})^{N+1}-\frac{(RHS_i^{\,w})^{N}}{(C_i^{\,w})^{N}}(C_i^{\,w})^{N+1/2} \quad \left(\text{if } (RHS_i^{\,w})^{N}<0\right) \qquad i\in[1,N_c]$$

where

$$(RHS_i^{\,w}) = \sum_{m=1}^{N_{rx}}(a_{mj}-b_{mj})k_m^{rb}h\left[\prod_{j=1}^{N_c}(C_j^{\,w})^{b_{mj}}-\frac{k_m^{rf}}{k_m^{rb}}\prod_{j=1}^{N_c}(C_j^{\,w})^{a_{mj}}\right]$$

$$+\left[M_i^{cw}+hk_i^{ab}p_i+\sum_{n=1}^{N_s}k_{ni}^{sb}S_n h C_{ni}^{\,s}+\sum_{n=1}^{N_s}k_{ni}^{bb}M_n C_{ni}^{\,b}+M_i^{crw}-M_j^{ciw}\right] \tag{3.241}$$

$$-\left[\lambda_i^{w}h+hk_i^{af}+\sum_{n=1}^{N_s}S_n hk_{ni}^{sf}+\sum_{n=1}^{N_s}M_n k_{ni}^{bf}+SS+R-I\right]C_i^{\,w} \qquad i\in[1,N_c]$$

For particulate chemicals on suspended sediments:

$$h\frac{(S_n C_{ni}^{\,s})^{N+1}-(S_n C_{ni}^{\,s})^{N+1/2}}{\delta t}$$

$$= (RHS_{ni}^{\,s})^{N+1}-(RHS_{ni}^{\,s})^{N} \quad \left(\text{if } (RHS_{ni}^{\,s})^{N}\geq 0\right) \tag{3.242}$$

$$= (RHS_{ni}^{\,s})^{N+1}-\frac{(RHS_{ni}^{\,s})^{N}}{(C_{ni}^{\,s})^{N}}(C_{ni}^{\,s})^{N+1/2} \quad \left(\text{if } (RHS_{ni}^{\,s})^{N}<0\right) \qquad n\in[1,N_s],\ i\in[1,N_c]$$

where

$$(RHS_{ni}^{\,s}) = \left[M_{ni}^{cs}+k_{ni}^{sf}hS_n C_i^{\,w}+R_n C_{ni}^{\,b}-D_n C_{ni}^{\,s}\right]-\left[\lambda_{ni}^{s}h+k_{ni}^{sb}h+SS+R-I\right]S_n C_{ni}^{\,s} \tag{3.243}$$

$$n\in[1,N_s],\ i\in[1,N_c]$$

(c) Solve Eqs. (3.241), (3.243), and (3.238) node by node with the Newton-Raphson method.

*Note: In Eqs. (3.235), (3.237), and (3.238) S_n and M_n are computed in Step 1, while h, **K**, reaction rate constants, stoichiometry, 1-st order decay constants, partial atmospheric pressure, and sources/sinks are either given or determined after the flow equations are solved.*

To achieve the (c) of Step 3, the following residual equations are constructed.

For dissolved chemicals:

$$(RES_i^w)$$

$$= h\left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2}\right] - \delta t\left[(RHS_i^w)^{N+1} - (RHS_i^w)^N\right] \quad \left(\text{if } (RHS_i^w)^N \geq 0\right)$$

$$= h\left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2}\right] - \delta t\left[(RHS_i^w)^{N+1} - \frac{(RHS_i^w)^N}{(C_i^w)^N}(C_i^w)^{N+1/2}\right] \quad \left(\text{if } (RHS_i^w)^N < 0\right) \tag{3.244}$$

$$i \in [1, N_c]$$

For particulate chemicals on suspended sediments:

$$(RES_{ni}^s)$$

$$= h\left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}\right] - \delta t\left[(RHS_{ni}^s)^{N+1} - (RHS_{ni}^s)^N\right] \quad \left(\text{if } (RHS_{ni}^s)^N \geq 0\right)$$

$$= h\left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}\right] - \delta t\left[(RHS_{ni}^s)^{N+1} - \frac{(RHS_{ni}^s)^N}{(C_{ni}^s)^N}(C_{ni}^s)^{N+1/2}\right] \quad \left(\text{if } (RHS_{ni}^s)^N < 0\right) \tag{3.245}$$

$$n \in [1, N_s], \quad i \in [1, N_c]$$

For particulate chemicals on bed sediments:

$$(RES_{ni}^b) = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t\,(RHS_{ni}^b)^{N+1} \qquad n \in [1, N_s], \quad i \in [1, N_c] \tag{3.246}$$

The associated Jacobian elements are thus computed as shown in the following.

For dissolved chemicals:

$$\frac{\partial(RES_i^w)}{\partial(C_l^w)^{N+1}} = \delta_{il} h + \delta_{il}\,\delta t\left[\lambda_i^w h + SS + R - I + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf}\right] -$$

$$\delta t\left[\sum_{m=1}^{N_{rx}} (a_{mi} - b_{mi}) h\left(k_m^{rb} b_{ml} (C_l^w)^{b_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^w)^{b_{mj}} - k_m^{rf} a_{ml} (C_l^w)^{a_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^w)^{a_{mj}}\right)\right] \tag{3.247}$$

$$i \in [1, N_c]$$

$$\frac{\partial(RES_i^w)}{\partial(C_{nl}^s)^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sb} S_n h \qquad n \in [1, N_s], \quad i \in [1, N_c], \tag{3.248}$$

$$\frac{\partial(RES_i^w)}{\partial(C_{nl}^b)^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{bb} M_n \qquad n \in [1, N_s], \quad i \in [1, N_c] \tag{3.249}$$

For particulate chemicals on suspended sediments:

$$\frac{\partial(RES_{ni}^{s})}{\partial(C_1^{w})^{N+1}} = -\delta_{il}\,\delta t\,k_{ni}^{sf}S_n h \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.250}$$

$$\frac{\partial(RES_{ni}^{s})}{\partial(C_{nl}^{s})^{N+1}} = \delta_{il}hS_n + \delta_{il}\,\delta t\,D_n + \delta_{il}\,\delta t\,S_n\left[\lambda_{ni}^{s}h + k_{ni}^{sb}h + SS + R - I\right] \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.251}$$

$$\frac{\partial(RES_{ni}^{s})}{\partial(C_{nl}^{b})^{N+1}} = -\delta_{il}\,\delta t\,R_n \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.252}$$

For particulate chemicals on bed sediments:

$$\frac{\partial(RES_{ni}^{b})}{\partial(C_1^{w})^{N+1}} = -\delta_{il}\,\Delta t\,k_{ni}^{bf}M_n \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.253}$$

$$\frac{\partial(RES_{ni}^{b})}{\partial(C_{nl}^{s})^{N+1}} = -\delta_{il}\,\Delta t\,D_n \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.254}$$

$$\frac{\partial(RES_{ni}^{b})}{\partial(C_{nl}^{b})^{N+1}} = \delta_{il}M_n + \delta_{il}\,\Delta t\,R_n + \delta_{il}\,\Delta t\,M_n\left[\lambda_{ni}^{b} + k_{ni}^{bb}\right] \qquad n\in[1,N_s],\ \ i\in[1,N_c] \tag{3.255}$$

4. EXAMPLES

In this section, we present the application of our model to solving a number of examples concerning (1) 1-D river/stream flow, (2) 2-D overland flow, (3) 1-D river/stream transport, (4) 2-D overland transport, (5) 1-D river/stream flow and transport, (6) 2-D overland flow and transport, (7) 1-D/2-D flow, and (8) 1-D/2-D flow and transport. Unless specifically announced, the diffusion wave model is solved when the simulation of water flow is involved in those examples.

4.1. Examples of 1-D river/stream flow

4.1.1. Example 1 of 1-D river/stream flow

In this example, a horizontally 200 m-long river/stream containing a uniform width of 2 m is considered. The bottom elevation of the river/stream is shown in Figure 4.1. Manning's roughness is 0.015. Initially, it is dry everywhere. As the simulation starts, a uniform rainfall of 10^{-5} m/s covers the entire domain of interest. At the upstream boundary node (i.e., X = 0 m) water depth is set at 10^{-10} m, while at the downstream boundary node (i.e., X = 200 m) a water depth-dependent flow rate boundary condition is applied. No infiltration is considered in this example. The domain is discretized with twenty elements, 10 m long for each. A one-hour simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop.

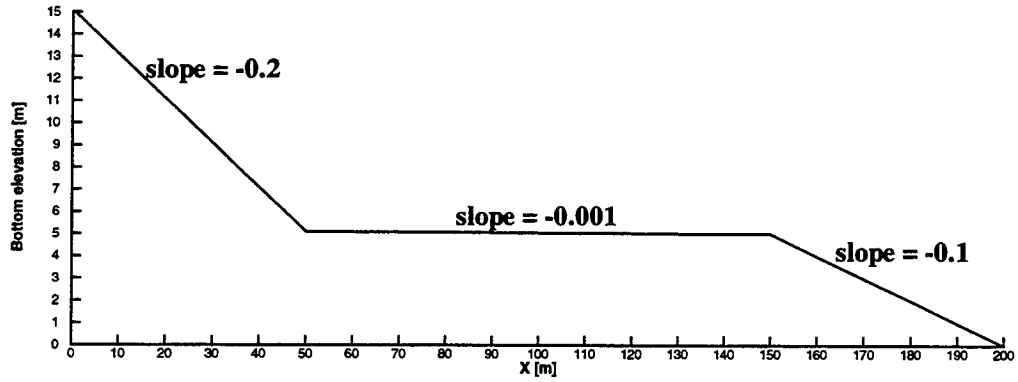

Figure 4.1. The bottom elevation of Example 1 of 1-D river/stream flow.

Figures 4.2 and 4.3 plot water depth and discharge, respectively, at time = 100 s, 200 s, 300 s, 600 s, and 1200 s. Since the change of water depth is almost unobservable after time = 1200 s, a steady state is presumed to have reached thereafter under a uniform rainfall of 10^{-5} m/s. From Figure 4.2, a hydraulic jump is observed from X = 50 m to X = 60 m due to the slope change from -0.2 to - 0.001. In each constant slope region (i.e., X = 0 to 50 m, X = 50 to 150 m, and X = 150 to 200 m), water depth has the tendency to increase gradually along the downslope direction because of a constant rainfall over the entire domain. We can also observe backwater effect in the region close to the downstream outlet (X = 170 to 200 m). In Figure 4.3, Discharge is computed by multiplying flow velocity with cross-sectional area which is water depth-dependent.

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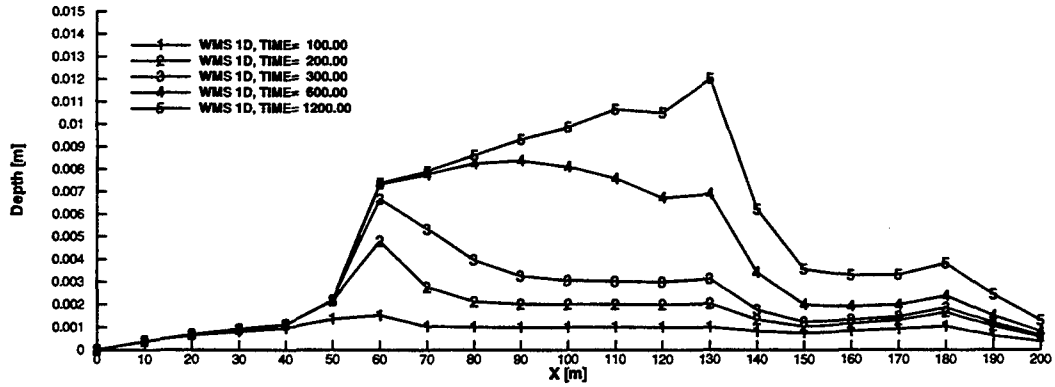


Figure 4.2. Water depth at various times for Example 1 of 1-D river/stream flow.

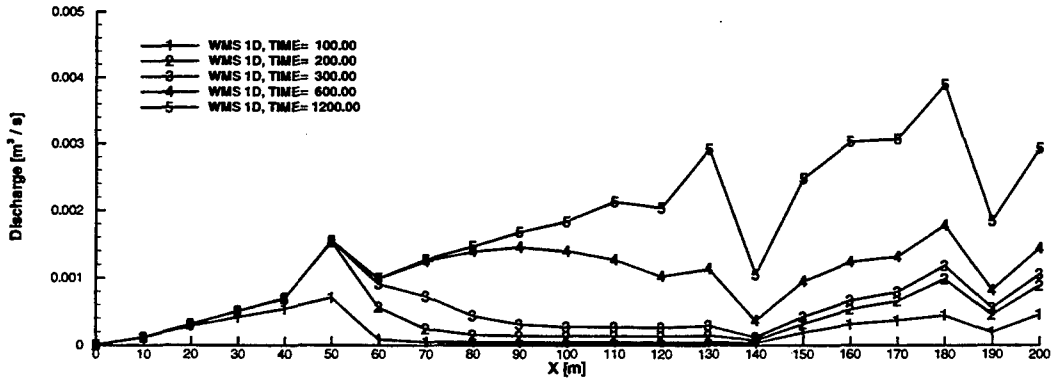


Figure 4.3. Discharge at various times for Example 1 of 1-D river/stream flow.

4.1.2. Example 2 of 1-D river/stream flow

This example simulates water flow in a river/stream network system. The system is composed of three river/stream reaches that are connected through a junction (Figure 4.4). Each reach is 100 m long and is discretized with 11 nodes and 10 elements: Nodes 1 through 11 for Reach 1, 12 through 22 for Reach 2, and 23 through 33 for Reach 3. Nodes 11, 12, and 33 coincide with one another and are located at the junction. The junction covers the area between Nodes 10 and 11, Nodes 12 and 13, and Nodes 32 and 33.

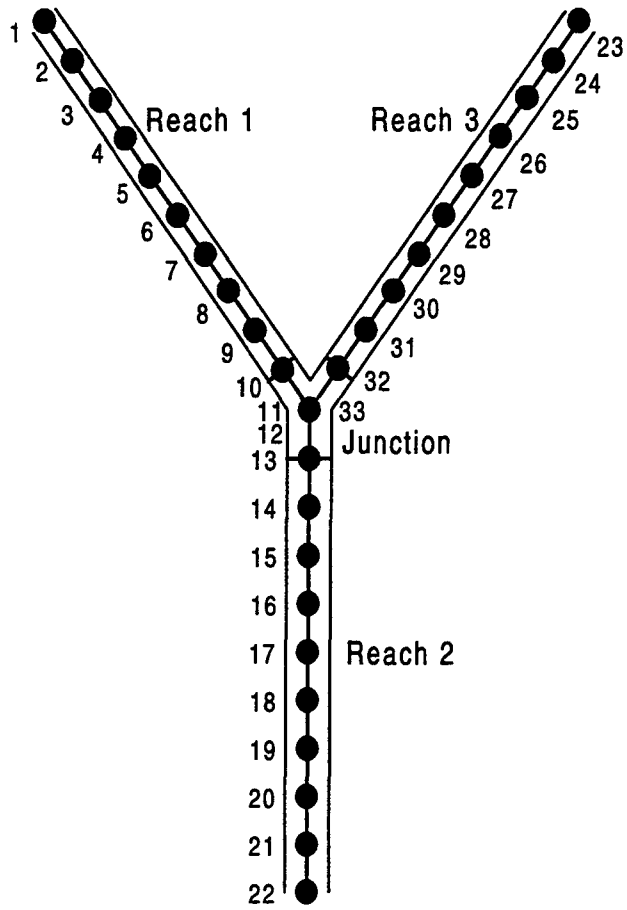


Figure 4.4. River/stream network for Example 2 of 1-D river/stream flow.

Reaches 1 and 3 have a uniform river/stream width of 2 m and the slope of their bottom elevation is -0.2 along the downstream direction, while Reach 2 contains a uniform river/stream width of 3 m and the slope of its bottom elevation is -0.1. Manning's roughness is 0.02 for all three reaches. Initially, it is dry everywhere. As the simulation starts, a uniform rainfall of 10^{-5} m/s is put on Reach 1. At Node 1 water depth is kept at 0 m, while a constant flow of $2x10^{-4}$ m^3/s flows through Node 23 through the simulation and a water depth-dependent flow rate boundary condition is applied at the downstream boundary node (i.e., Node 22). No infiltration is considered in this example. A one-hour simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop.

Figures 4.5 through 4.7 plots water depth at various times for Reaches 1 through 3, respectively. Since rainfall and upstream boundary conditions do not vary with time, a steady state is observed after time = 600 s. It is noted that the downstream node of Reach 1 (i.e., at X = 100 m in Figure 4.5), the upstream node of Reach 2 (i.e., at X = 0 m in Figure 4.6) and the downstream node of Reach 3 (i.e., at X = 100 m in Figure

4.7) coincide with one another and are where the junction is. One can verify this by checking the water depths at these locations. We can see the marching of wet fronts in both Figures 4.6 and 4.7 and an increasing depth along the downstream direction in Figure 4.5 due to a constant uniform rainfall.

For the 1-st reach

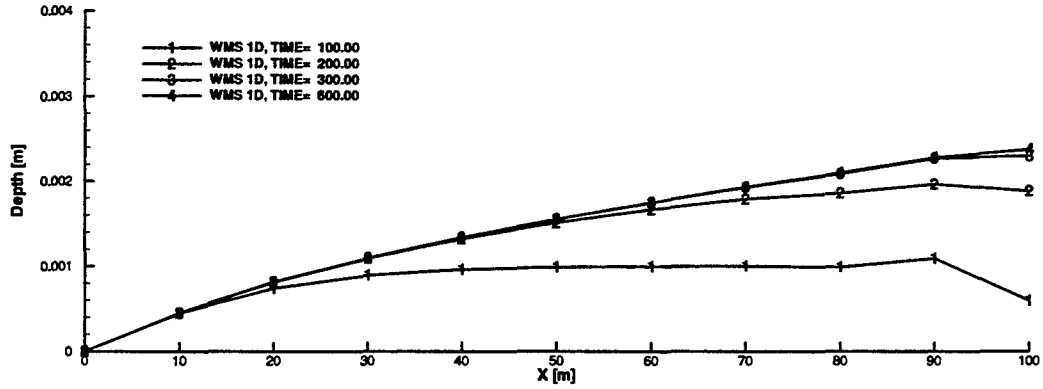


Figure 4.5. Water depth of Reach 1 at various times for Example 2 of 1-D river/stream flow.

For the 2-nd reach

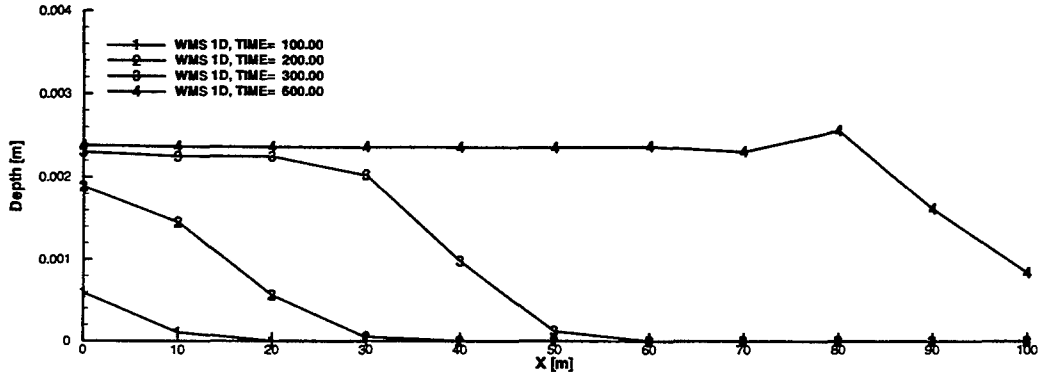


Figure 4.6. Water depth of Reach 2 at various times for Example 2 of 1-D river/stream flow.

For the 3-rd reach

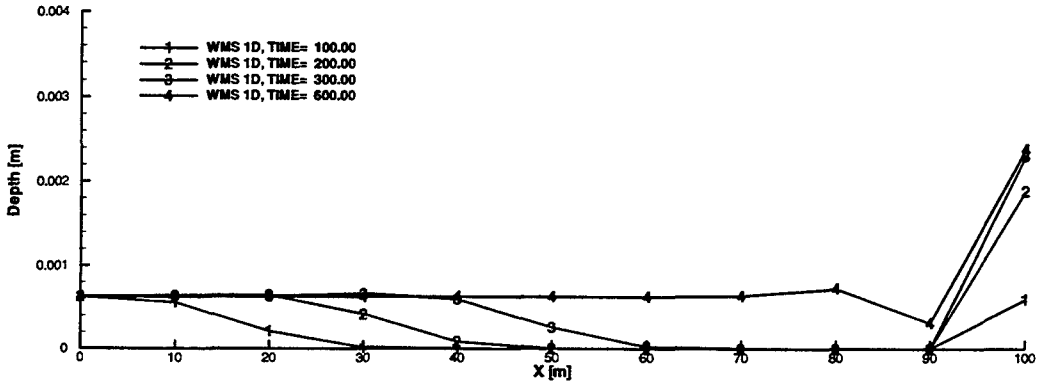


Figure 4.7. Water depth of Reach 3 at various times for Example 2 of 1-D river/stream flow.

4.2. Example of 2-D overland flow

Two examples are presented in this subsection. Example 1 is to show the application of using the diffusion wave model to handle an overland system which contains the slope of bottom elevation ranging from 0.01 to 0.5; Because of the steep slope involved, the dynamic model is difficult to solve with any numerical scheme, even with the most physically natural method of characteristics. Example 2 is a standing wave problem to demonstrate the capability of the method of characteristics to accurately solve the dynamic wave model when the slope is small. Difficulty is encountered in dealing with water flow over steep slope overland system by solving the dynamic wave model. On the other hand, the diffusion wave model cannot provide accurate solution when the inertia terms are important, such as flow on a flat region. Thus, it is desirable to develop a hybrid model in which an adaptive scheme can be built to automatically select appropriate models (kinematic, diffusion, or dynamic wave models) for different regions of the entire watershed.

4.2.1. Example 1 of 2-D overland flow

The domain of interest coveres a horizontal area of 200 m x 80 m. The bottom elevation contour is given in Figure 4.8. The domain is discretized with 320 triangular elements (Figure 4.9). Manning's roughness is 0.04. Initially, it is dry everywhere. A two-hour simulation is performed with a fixed time step size of 5 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop. As the simulation starts, a uniform rainfall of 10^{-5} m/s covers the entire domain of interest for the first half hour and 1.5×10^{-5} m/s for the third half hour. As for the second and the fourth half hours, the rainfall rate is zero. On the upstream boundary side (i.e., X = 0 m) water depth is set at 10^{-10} m through the simulation, while on the downstream boundary side (i.e., X = 200 m) a water depth-dependent flux boundary condition is applied. The boundaries of Y = 0 m and 80 m are impermeable. No infiltration is considered in this example.

Figure 4.10 plots water depth at various times from the simulation. From the figure, we can first see the irregular depth distribution due to the slope change of ground surface (Figure 4.8). Since the water depths at Time = 600 s, 1200 s, and 1800 s can not be distinguished, we may say a steady state has reached by Time = 600 s under a rainfall of 10^{-5} m/s. Likewise, the depths at the end of the second and the fourth half hours (i.e., Time = 3600 s and 7200 s, respectively) tells us the steady state for the two non-rainfall period of times have reached by then.

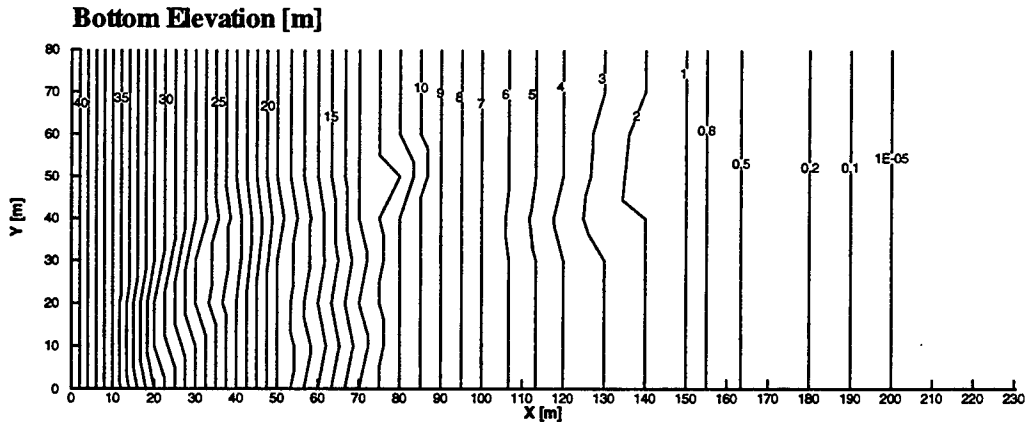


Figure 4.8. The contour of bottom elevation for Example 1 of 2-D overland flow.

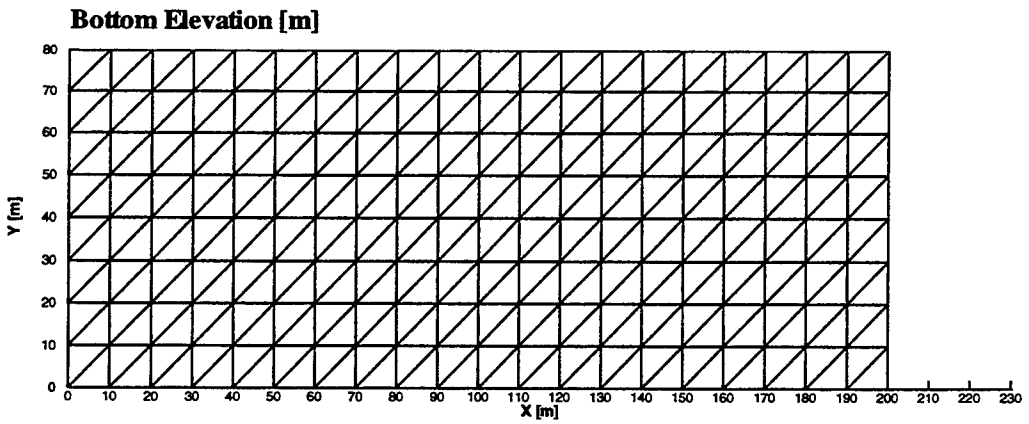


Figure 4.9. Discretization for Example 1 of 2-D overland flow.

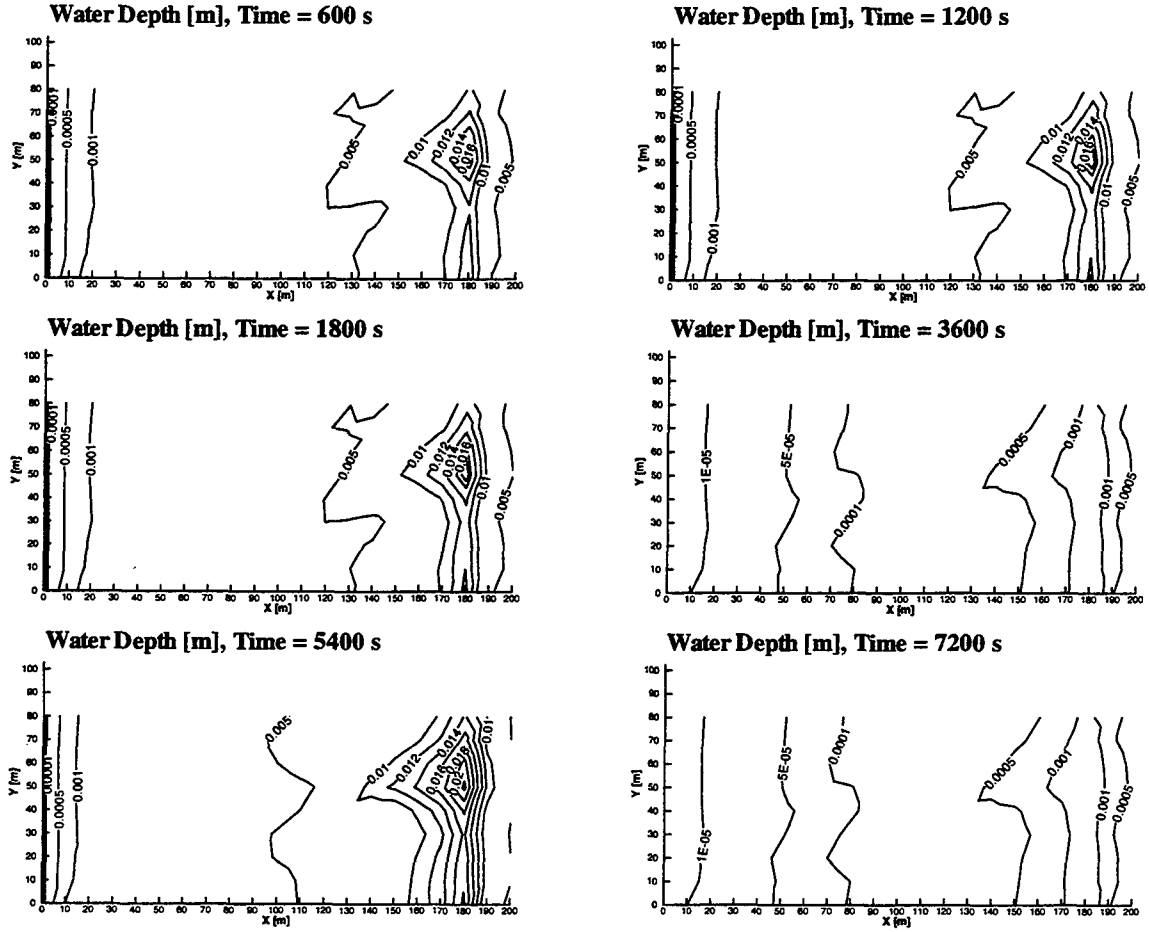


Figure 4.10. Water depth at various times for Example 1 of 2-D overland flow.

4.2.2. Example 2 of 2-D overland flow

A 1-D standing wave problem is considered in this example. It is solved by 2-D method of characteristics, as presented in Section 3.2.1. This problem is governed by the wave equations as follows.

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{4.1}$$

$$\frac{\partial^2 \eta}{\partial t^2} = c^2 \frac{\partial^2 \eta}{\partial x^2} \tag{4.2}$$

$$c^2 = gh \tag{4.3}$$

where u is the velocity along the 1-D direction [L/T]; c is the wave speed [L/T]; h is water depth [L]; η is stage deviation [L]; g is gravity [L/T^2]. The domain of interest is 200 m long in the x-direction and 50 m wide in the y-direction. It is discretized with 20 elements: 10 m x 50 m each. The boundary end of X = 200 m is closed, while the other one at X = 0 m is open and the water stage is forced up and down according to

$$\eta|_{X=0m} = \frac{1}{10}\sin\frac{2\pi t}{200} \tag{4.4}$$

Thus, we set u = 0 m/s at X = 200 m to settle the boundary condition for achieving the simulation. The analytical solution of this problem can be found as follows [Wang and Connor, 1975].

$$u = -\frac{a\sqrt{c}}{h\cos\frac{2\pi}{\sqrt{c}}}\sin\left[\frac{2\pi}{\sqrt{c}}\left(\frac{x}{200}-1\right)\right]\cos\frac{2\pi t}{200} \quad \text{m/s} \tag{4.5}$$

$$\eta = -\frac{a}{\cos\frac{2\pi}{\sqrt{c}}}\cos\left[\frac{2\pi}{\sqrt{c}}\left(\frac{x}{200}-1\right)\right]\sin\frac{2\pi t}{200} \quad \text{m} \tag{4.6}$$

A simulation of 400 seconds is performed, where time step size is set to 2.5 seconds. The initial condition is given at t = 50 s according to Eqs. (4.5) and (4.6). Figures 4.11 and 4.12 show the comparison of water depth and velocity, respectively, between analytical solution and computed results at various times. The comparison simply tells that the method of characteristics can solve the dynamic wave model quite accurately.

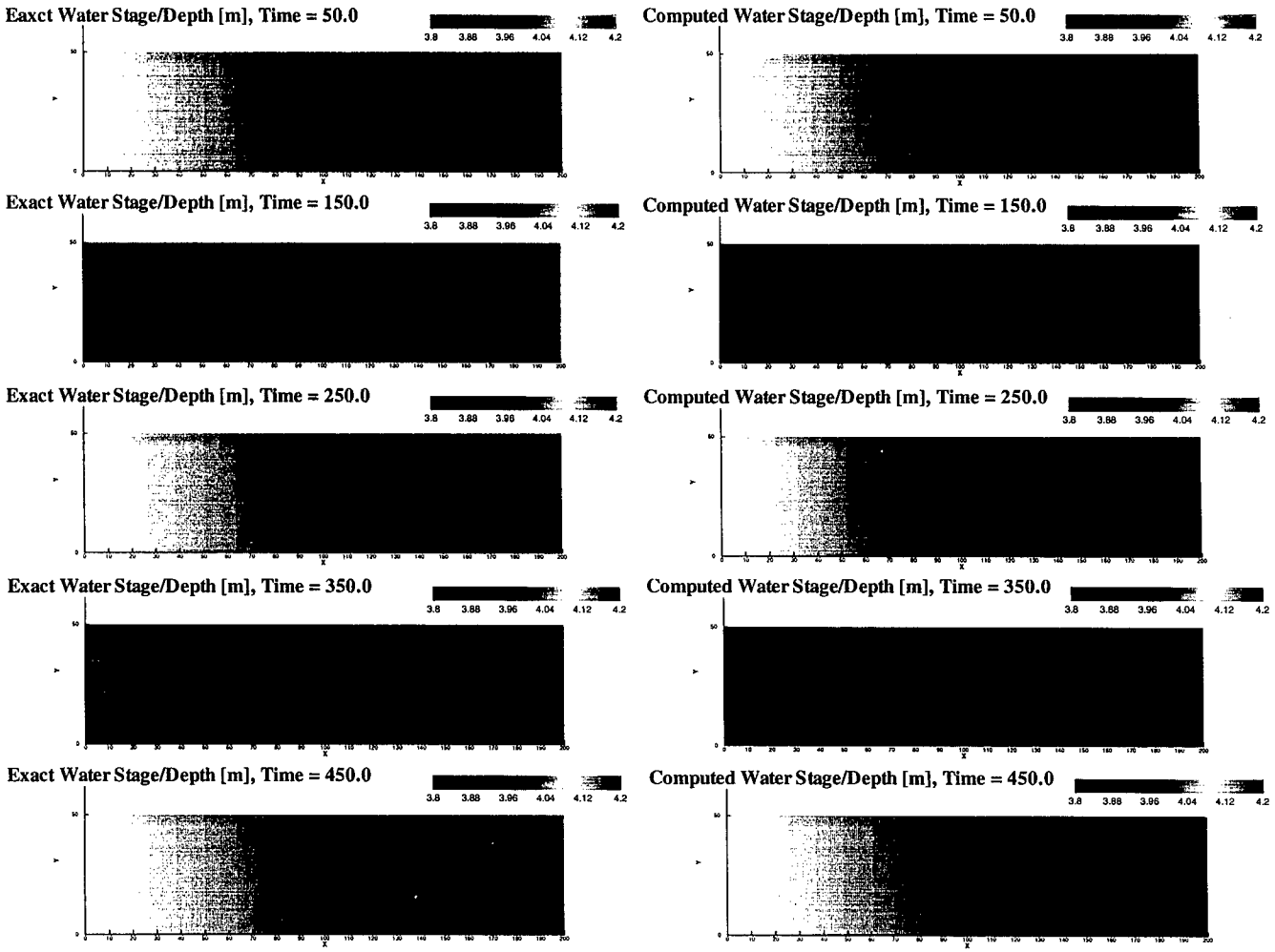


Figure 4.11. Comparison of water depth between analytical solutions and numerical results for Example 2 of 2-D overland flow.

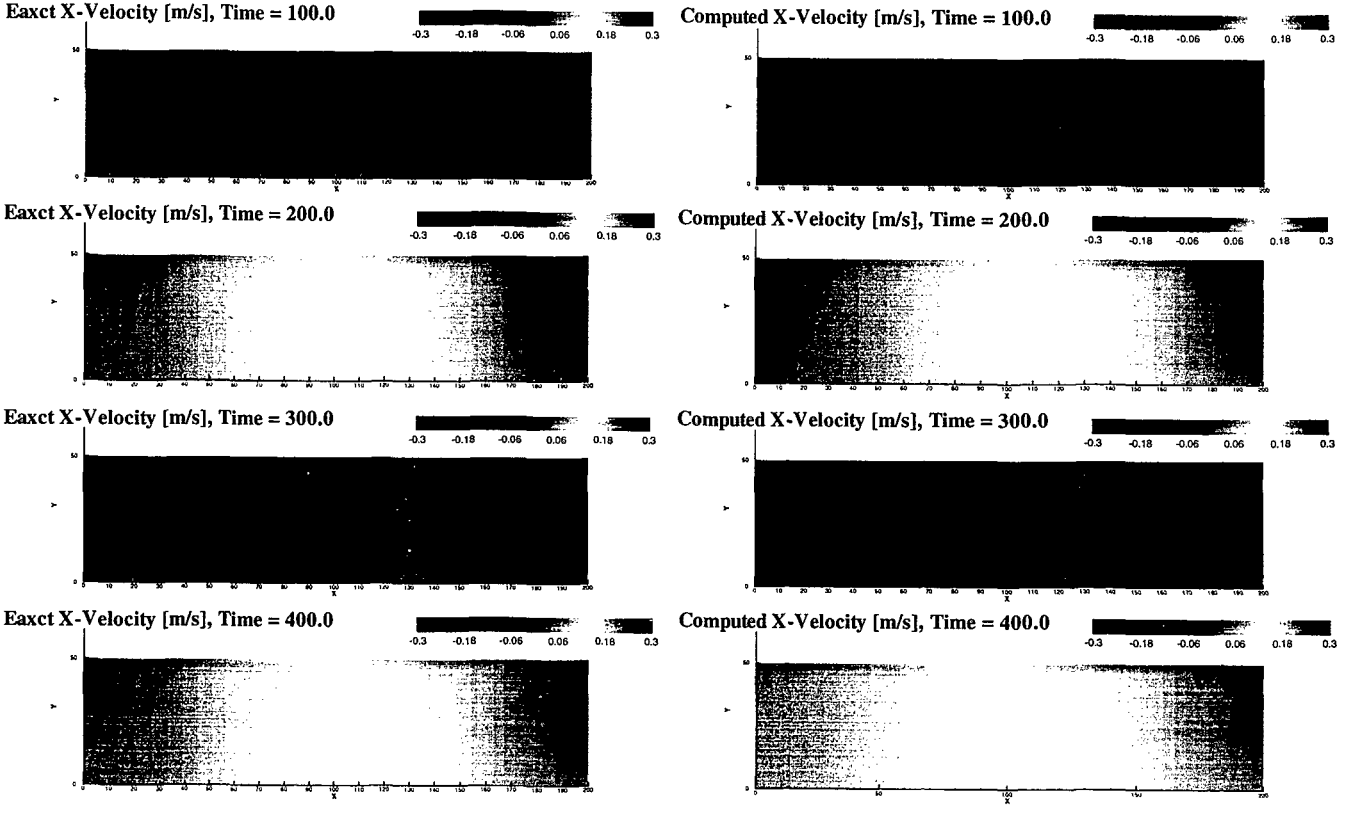


Figure 4.12. Comparison of velocity between analytical solutions and numerical results for Example 2 of 2-D overland flow.

4.3. Example of 1-D river/stream transport

This example is to demonstrate the capability of the model in simulating both contaminant and sediment transport. A horizontally 200 m-long river/stream containing a uniform width of 2 m is considered. To focus on transport, we assume water depth is 2 m and river/stream velocity is 1 m/s throughout the river/stream. Three dissolved chemicals are considered to undergo the following reaction.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C3} \qquad k_f = 0.002, \quad k_b = 0.005 \tag{4.7}$$

where $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$ represent dissolved chemicals.

Three sizes of sediments are taken into account and are considered to be cohesive sediments. The settling speeds are $1.2\text{x}10^{-6}$ m/s for Sediment 1, $1.5\text{x}10^{-4}$ m/s for Sediment 2, and $4.5\text{x}10^{-2}$ m/s for Sediment 3. The critical shear stresses for deposition and erosion are 2.75 g/m/s^2 and 2.68 g/m/s^2, respectively, for all three sediments. The following sorption reactions are included.

$$\overline{CC} + \overline{SS1} \rightleftharpoons \overline{PS1} + \overline{SS1} \qquad k_f = 0.001, \quad k_b = 0.0 \tag{4.8}$$

$$\overline{CC} + \overline{SS2} \rightleftharpoons \overline{PS2} + \overline{SS2} \qquad k_f = 0.001, \quad k_b = 0.0 \tag{4.9}$$

$$\overline{CC} + \overline{SS3} \rightleftharpoons \overline{PS3} + \overline{SS3} \qquad k_f = 0.001, \quad k_b = 0.0 \tag{4.10}$$

$$\overline{CC} + \overline{BS1} \rightleftharpoons \overline{PB1} + \overline{BS1} \qquad k_f = 0.0001, \quad k_b = 0.0 \tag{4.11}$$

$$\overline{CC} + \overline{BS2} \rightleftharpoons \overline{PB2} + \overline{BS2} \qquad k_f = 0.0001, \quad k_b = 0.0 \tag{4.12}$$

$$\overline{CC} + \overline{BS3} \rightleftharpoons \overline{PB3} + \overline{BS3} \qquad k_f = 0.0001, \quad k_b = 0.0 \tag{4.13}$$

where $\overline{CC}$ can be $\overline{C1}$, $\overline{C2}$, or $\overline{C3}$; $\overline{SS1}$, $\overline{SS2}$, and $\overline{SS3}$ are suspended sediments; $\overline{BS1}$, $\overline{BS2}$, and $\overline{BS3}$ are bed sediments; $\overline{PS1}$, $\overline{PS2}$, and $\overline{PS3}$ are particulate chemicals on suspended sediments associated with $\overline{CC}$; $\overline{PB1}$, $\overline{PB2}$, and $\overline{PB3}$ are particulate chemicals on bed sediments associated with $\overline{CC}$. We have, therefore, 18 sorption reactions in total.

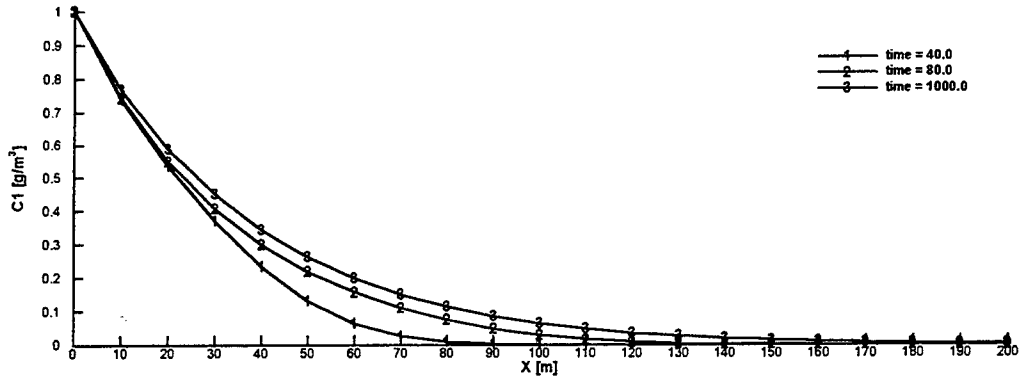
Initially, only bed sediments exist in the domain of interest. The initial concentration is 50 g/m^3 for

boundary conditions are applied to the upstream boundary node (i.e., X = 0 m), where all dissolved chemicals have a constant concentration of 1 g/m^3 and all other mobile materials have zero concentration at this boundary node. The longitudinal dispersivity is 0.01 m. A 1000 second simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for both linear and nonlinear iterations involved in the computation.

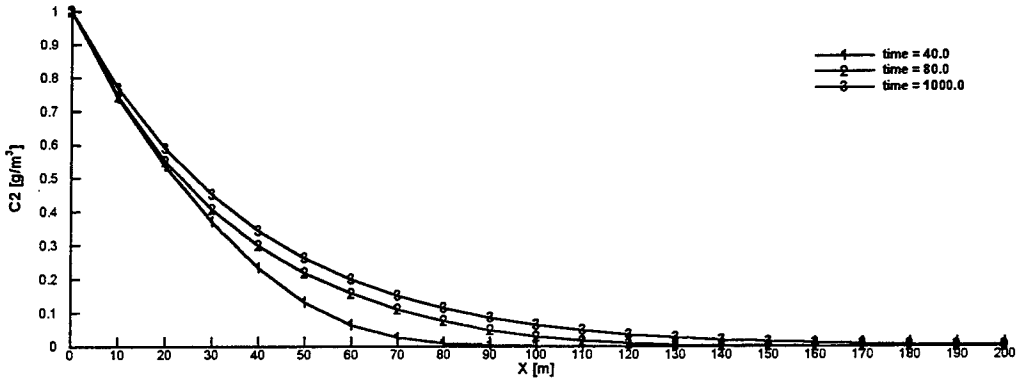
Figures 4.13 through 4.17 plot the numerical results at various time, including concentration distributions for (1) dissolved chemicals (Figure 4.13), (2) suspended sediments (Figure 4.14), (3) bed sediments (Figure 4.15), (4) particulate chemicals on suspended sediments (Figure 4.16), and (5) particulate chemicals on bed sediments (Figure 4.17). Since the first and second dissolved chemicals are involved in identical reactions, their concentration distributions are identical to each other, so do those of their related particulate chemicals.

Figure 4.13 shows a decreasing dissolved chemical concentration for all three dissolved chemicals. This is because we allow the adsorption to happen, but do not allow desorption from particulate chemicals to dissolved chemicals (see Eqs. (4.8) through (4.13)). Figure 4.14 shows the trend of increasing concentration of suspended sediment along the downstream direction, while Figure 4.15 depict the decrease of bed sediment with the increase of time. Figures 4.14 and 4.15 tell that the deposition is less than the erosion under the condition set for this example. Figures 4.16 and 4.17 also help verify this. Since the dissolved chemicals are little in the downstream region, the major source of chemicals are the particulate chemicals on suspended sediments that are transported from the upstream region along with water. Because erosion is greater than deposition, we can hardly find particulate chemicals on bed sediments in the downstream region (Figure 4.17). On the other hand, we observe an increase of particulate chemical on suspended sediments along the downstream direction (Figure 4.16). By comparing the numerical results at various times, it seems that the concentration distributions (Figures 4.13, 4.14, and 4.16) are approaching a steady state. This tendency will continue until the bed sediments are completely depleted, starting from the upstream end.

(a)



(b)



(c)

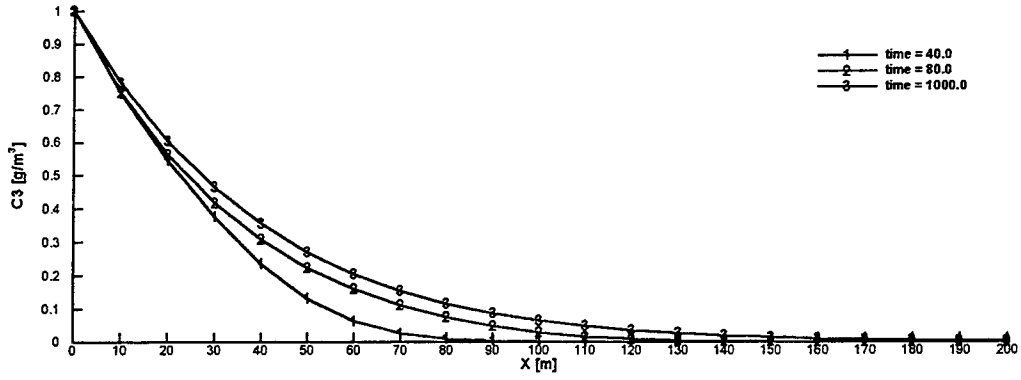
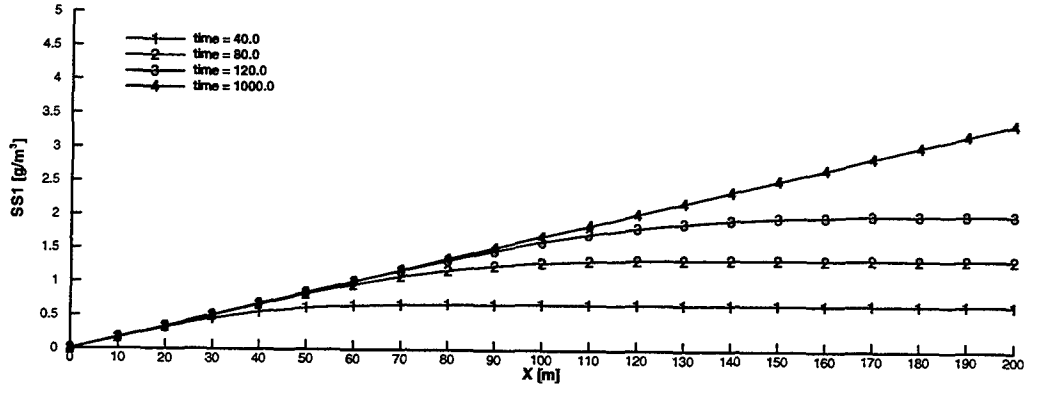
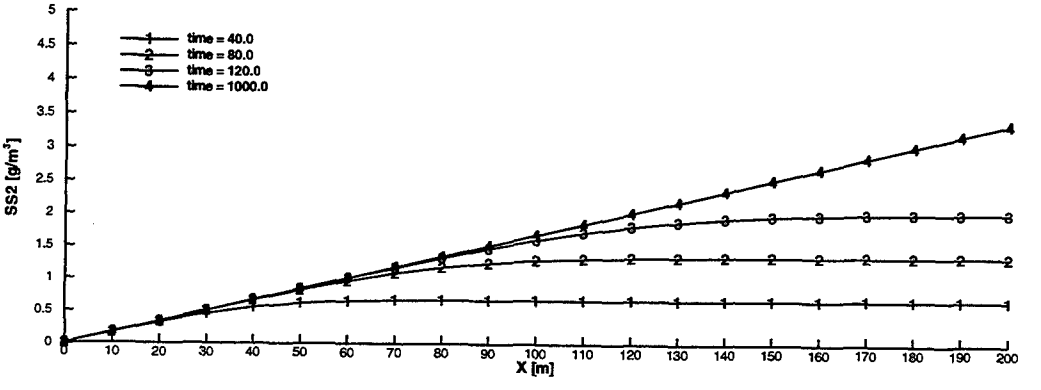


Figure 4.13. Concentrations of (a) the first, (b) the second, and (c) the third dissolved chemicals for the example of 1-D river/stream transport.

(a)



(b)



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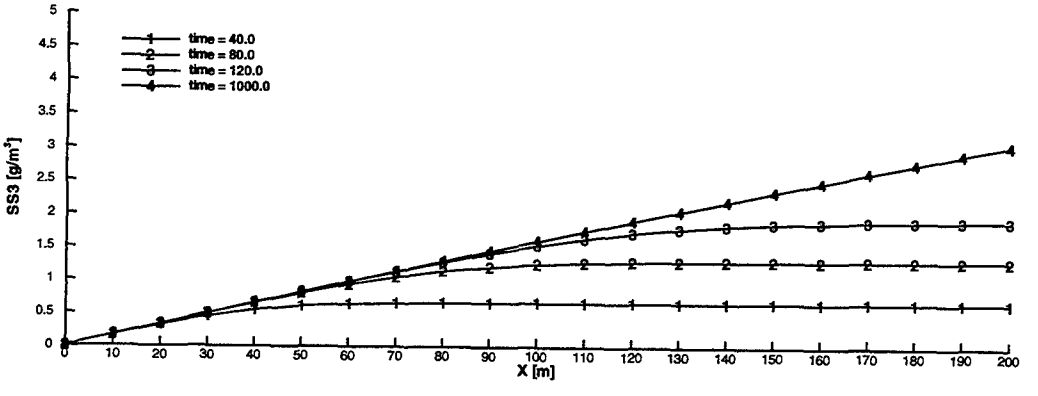
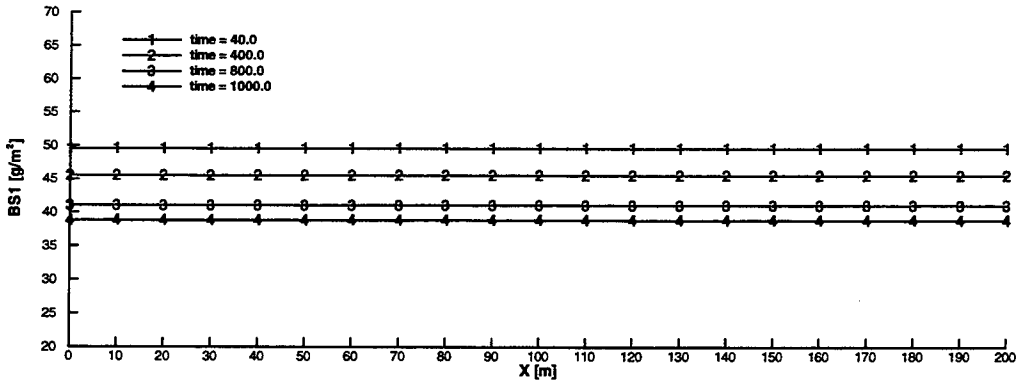
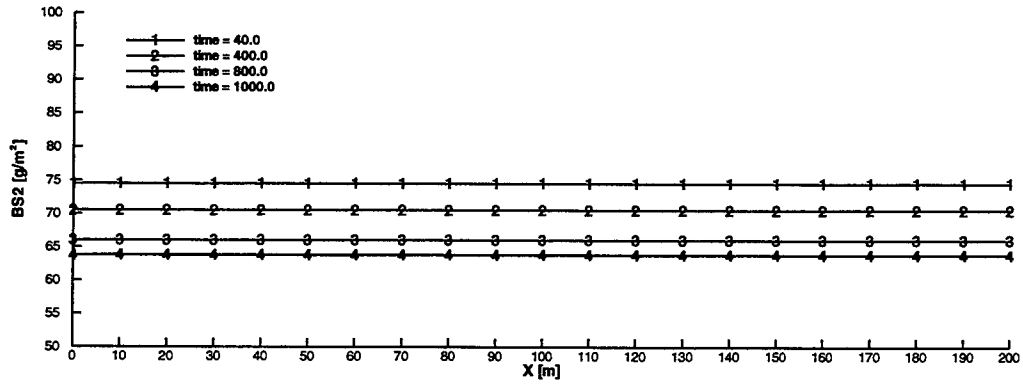


Figure 4.14. Concentrations of (a) the first, (b) the second, and (c) the third suspended sediments for the example of 1-D river/stream transport.

(a)



(b)



(c)

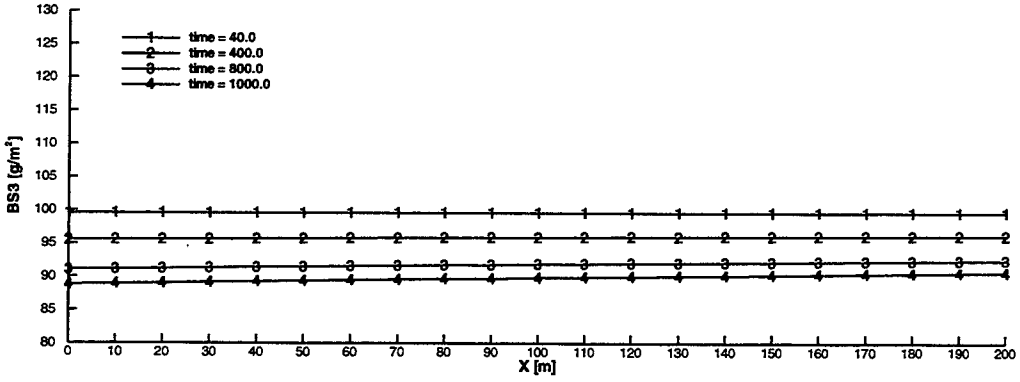
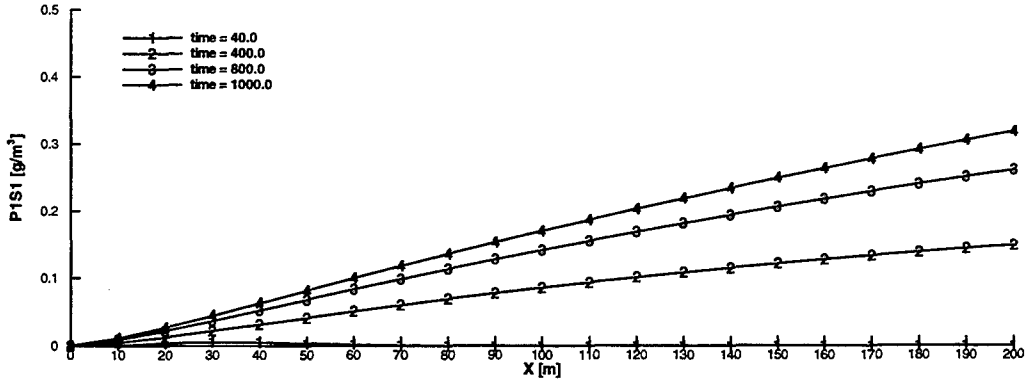
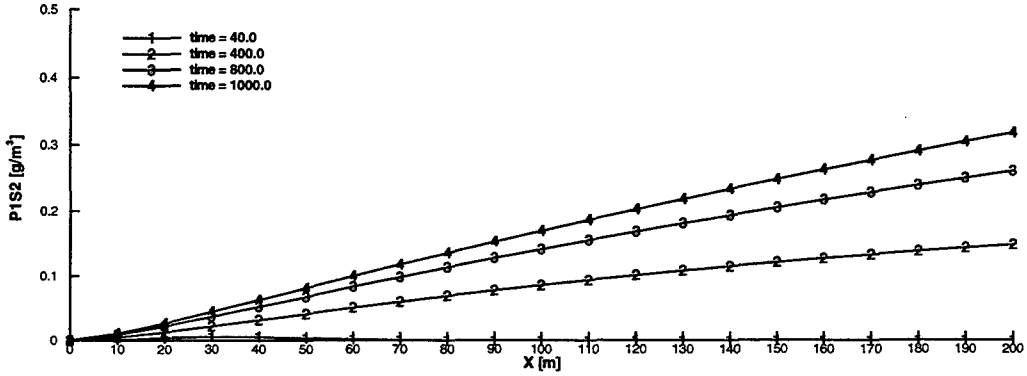


Figure 4.15. Concentrations of (a) the first, (b) the second, and (c) the third bed sediments for the example of 1-D river/stream transport.

(a)



(b)



(c)

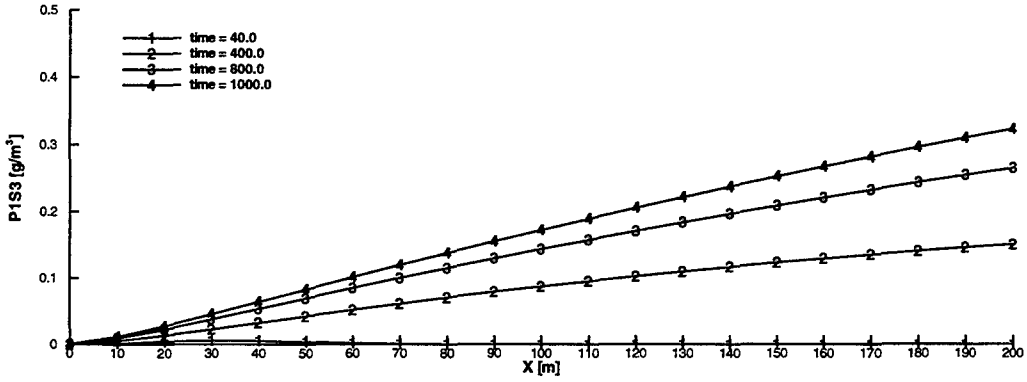
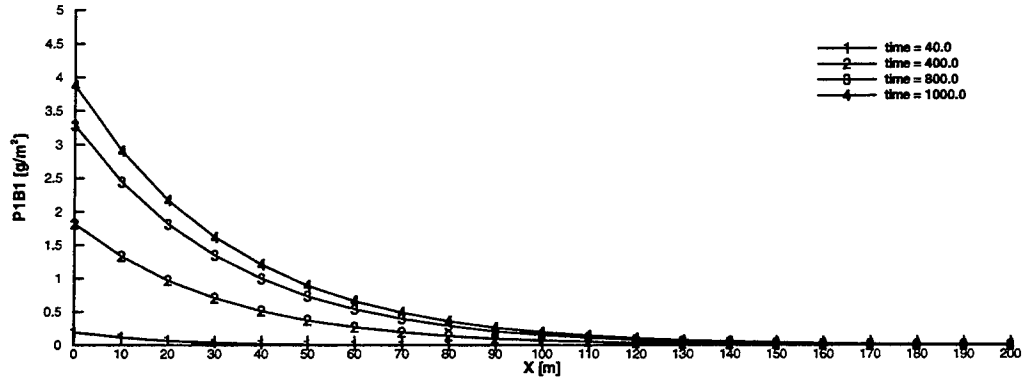
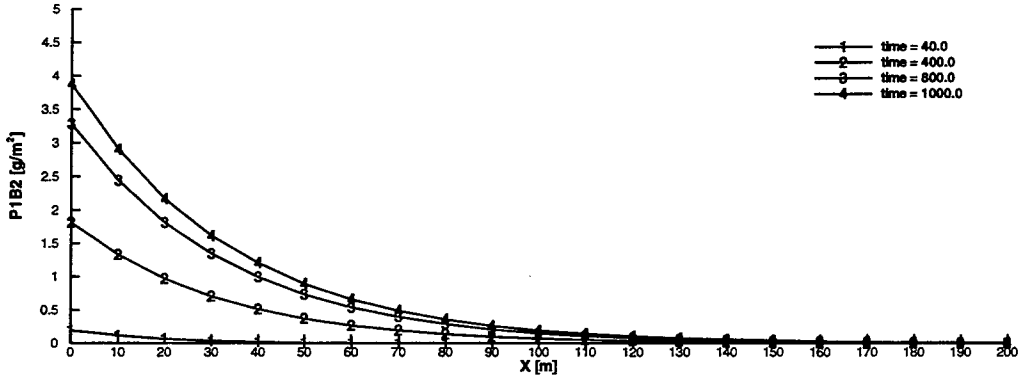


Figure 4.16. Concentrations of the first particulate chemical on (a) the first, (b) the second, and (c) the third suspended sediments for the example of 1-D river/stream transport.

(a)



(b)



(c)

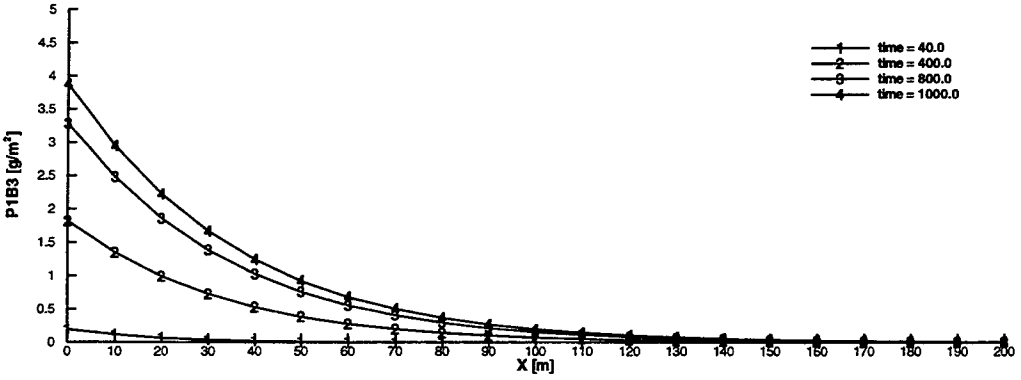


Figure 4.17. Concentrations of the first particulate chemical on (a) the first, (b) the second, and (c) the third bed sediments for the example of 1-D river/stream transport.

4.4. Example of 2-D overland transport

The domain of interest has covered a horizontal area of 200 m x 70 m and is discretized with 140 rectangular elements: 10 m x 10 m for each element. To deal with transport only, water depth is set to 1 m and the velocity is -1.0 m/s in the x-direction and 0.0 m/s in the y-direction everywhere. The following chemical reactions are embraced.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C4} \qquad k_f = 0.01, \quad k_b = 0.005 \tag{4.14}$$

$$\overline{C1} + \overline{C3} \rightleftharpoons \overline{C5} \qquad k_f = 0.01, \quad k_b = 0.0025 \tag{4.15}$$

$$\overline{C2} + 2\overline{C3} \rightleftharpoons \overline{C6} \qquad k_f = 0.01, \quad k_b = 0.001 \tag{4.16}$$

where $\overline{C1}$, $\overline{C2}$, $\overline{C3}$, $\overline{C4}$, $\overline{C5}$, and $\overline{C6}$ are dissolved chemicals.

Initially, there is no dissolved chemical anywhere in the domain. A 600 second simulation is performed with a fixed time step size of 10 seconds. A relative error of 10^{-4} is used to determine convergence for the nonlinear loop. As the simulation starts, a Dirichlet concentration of 1 g/m^3 is applied for $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$ on the upstream boundary (i.e., X = 200 m) between Y = 30 m and 40 m. The boundaries of Y = 0 m and 70 m are impervious. The longitudinal and transverse dispersivities are 0.5 m and 0.1 m, respectively. The diffusion coefficient is 10^{-5} m^2/s.

Figures 4.18 through 4.23 show the numerical result at time = 260 s. A steady state result is considered to have reached after 260 s. The maximum concentrations of $\overline{C4}$, $\overline{C5}$, and $\overline{C6}$ are 0.26286 g/m^3, 0.25637 g/m^3, and 0.16833 g/m^3, respectively, which are found in the middle of downstream area (i.e., X = 40 to 50 m and Y = 30 to 40 m)

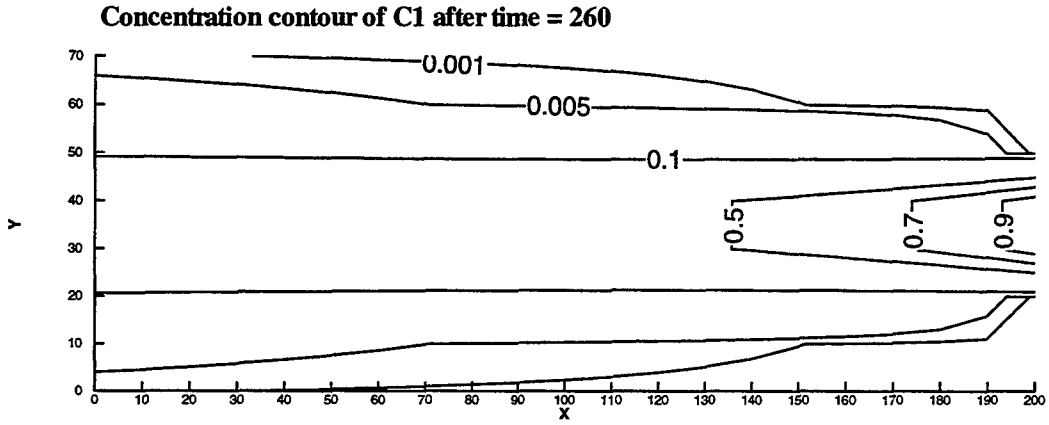


Figure 4.18. Concentration contour of the first dissolved chemical at time = 260 s for the example of 2-D overland transport.

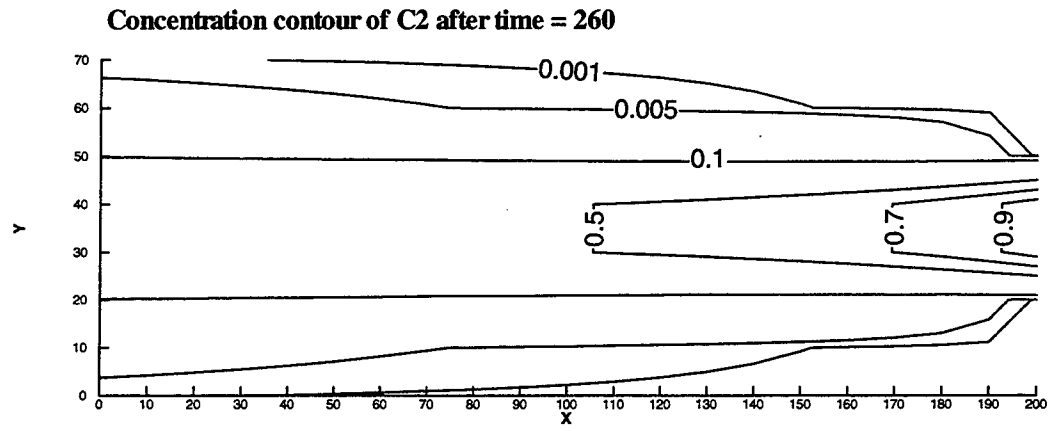


Figure 4.19. Concentration contour of the second dissolved chemical at time = 260 s for the example of 2-D overland transport.

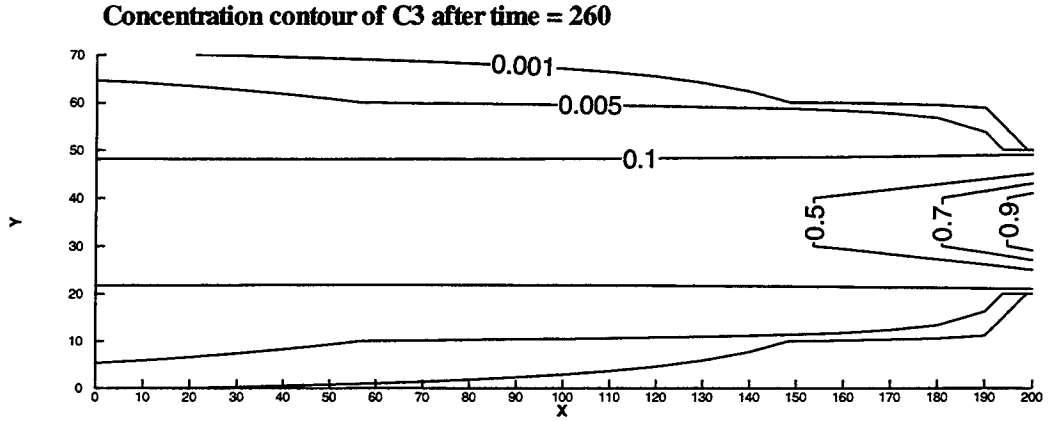


Figure 4.20. Concentration contour of the third dissolved chemical at time = 260 s for the example of 2-D overland transport.

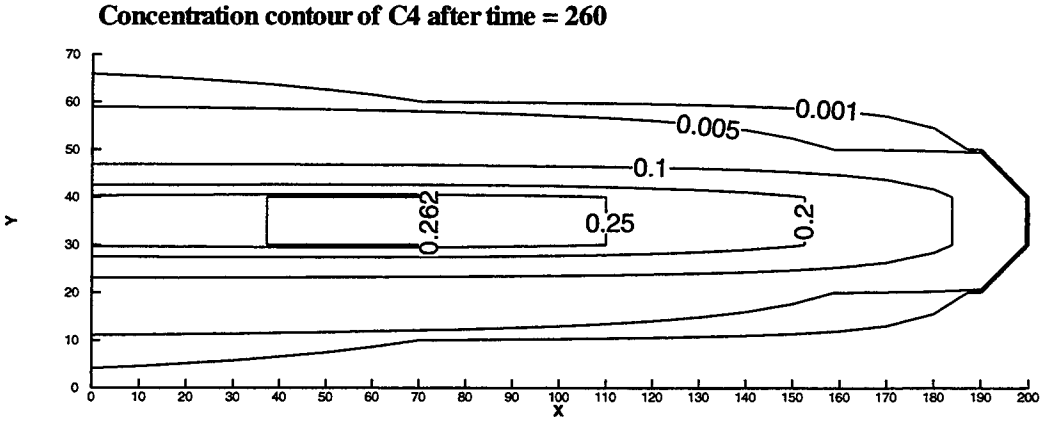


Figure 4.21. Concentration contour of the fourth dissolved chemical at time = 260 s for the example of 2-D overland transport.

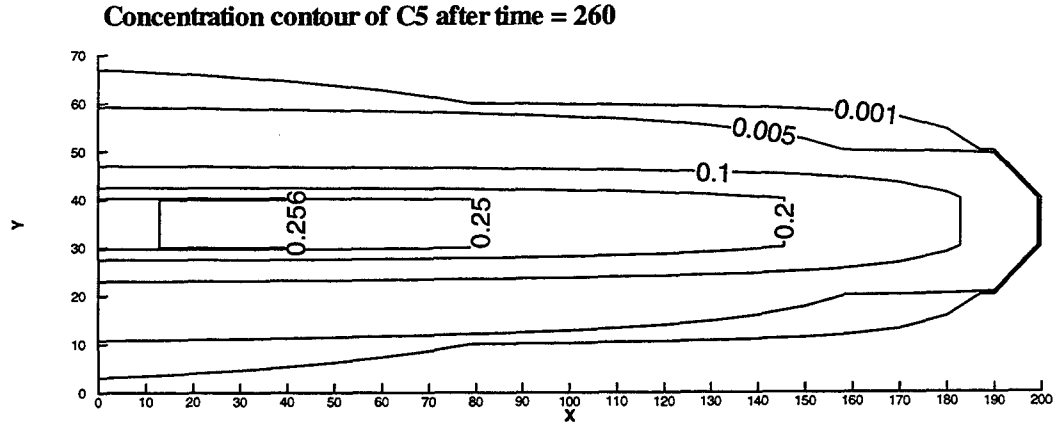


Figure 4.22. Concentration contour of the fifth dissolved chemical at time = 260 s for the example of 2-D overland transport.

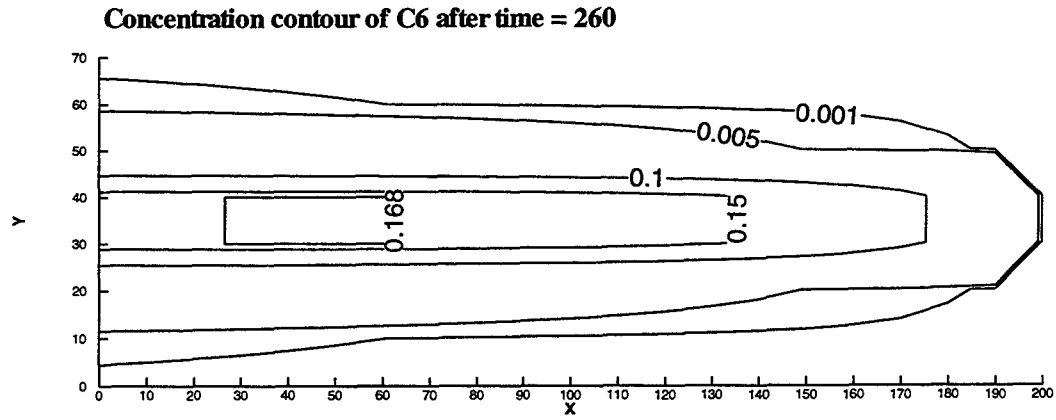


Figure 4.23. Concentration contour of the sixth dissolved chemical at time = 260 s for the example of 2-D overland transport.

4.5. Example of 1-D river/stream flow and transport

In this example, a horizontally 200 m-long river/stream containing a uniform width of 2 m is

considered. The bottom elevation of the river/stream is shown in Figure 4.1. Manning's roughness is 0.015. Initially, it is dry everywhere. The chemical reactions considered are identical to those in the example of 2-D transport (Eqs. (4.14) through (4.16)). As the simulation starts, a uniform rainfall of 10^{-5} m/s covers the entire domain of interest, which contains the first three chemicals (i.e., $\overline{C1}$, $\overline{C2}$, and $\overline{C3}$) of 1 g/m^3. At the upstream boundary node (i.e., X = 0 m) water depth is kept at 10^{-10} m and the concentrations are kept at 1 g/m^3 for $\overline{C1}$, $\overline{C2}$, $\overline{C3}$ and at 0 g/m3 for $\overline{C4}$, $\overline{C5}$, $\overline{C6}$. At the downstream boundary node (i.e., X = 200 m) a water depth-dependent flow rate boundary condition is employed for flow and a variable boundary condition is applied for transport. Infiltration is neglected. The domain is discretized with twenty elements, 10 m long for each. A one-hour simulation is performed with a fixed time step size of 2 seconds. A relative error of 10^{-4} is used to determine convergence for required iteration in both flow and transport computations.

Figure 4.24 depicts water depth at various times for the simulation. It is the same as Figure 4.2 because they have an identical setup for the flow simulation and we assume the flow is not influenced by transport in our model. Figures 4.25 through 4.31 show the concentration distributions at various times for the first through the sixth dissolved chemicals, respectively. It is seen that the third dissolved chemicals are consumed most among the three reactant chemicals that consumes most in this example (Figures 4.25 through 4.27). This is because all three reactions contain the same forward reaction rate constant (Eqs. (4.16) through (4.18)) but the third reaction has the smallest backward reaction rate constant and the third dissolved chemical has a stoichiometric coefficient of 2 as a reactant chemical in the third reaction (Eq. (4.16)).

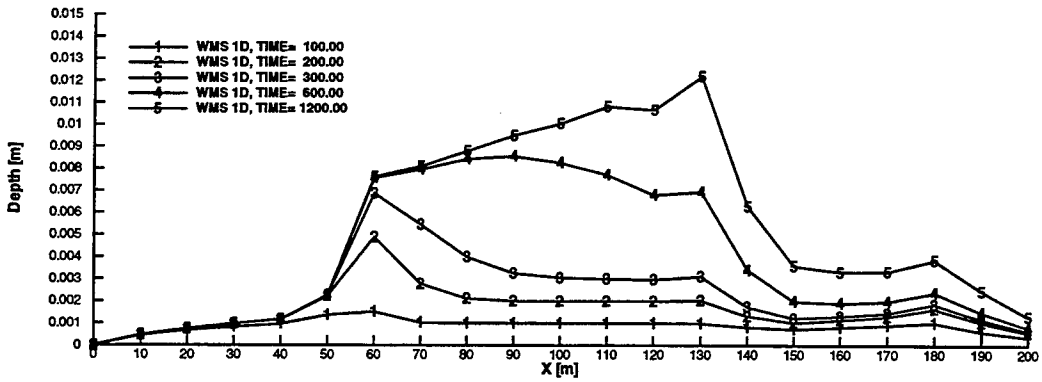


Figure 4.24. Water depth at various times for the example of 1-D river/stream flow and transport.

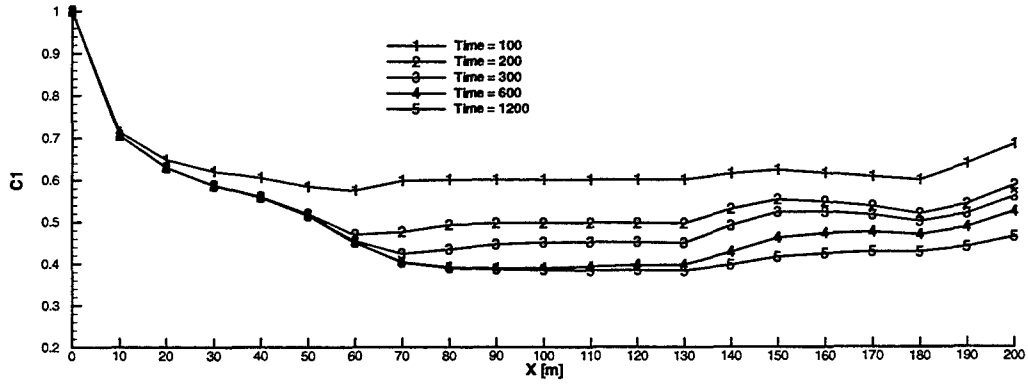


Figure 4.25. Concentration of the first dissolved chemical at various times for the example of 1-D river/stream flow and transport.

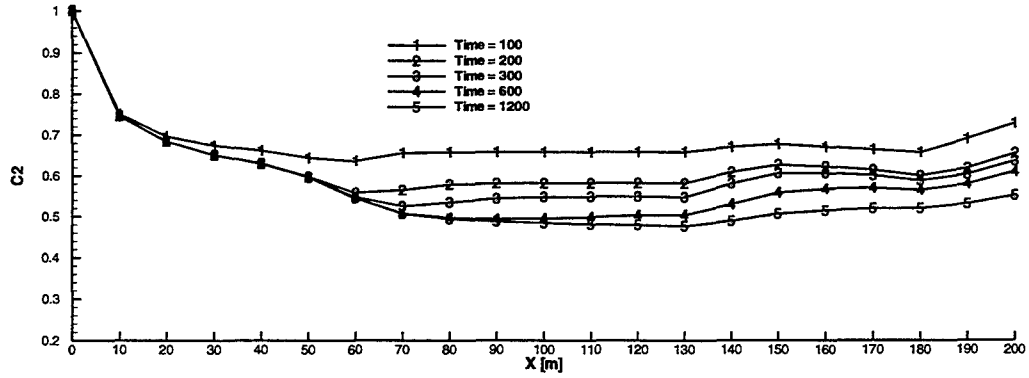


Figure 4.26. Concentration of the second dissolved chemical at various times for the example of 1-D river/stream flow and transport.

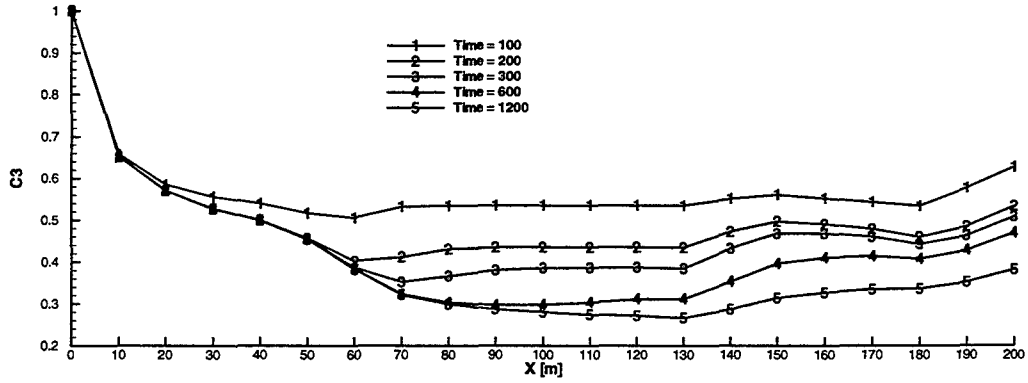


Figure 4.27. Concentration of the third dissolved chemical at various times for the example of 1-D river/stream flow and transport.

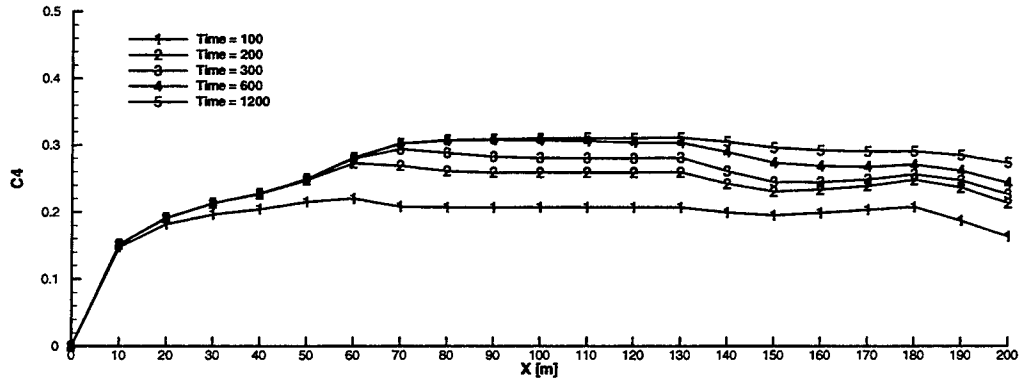


Figure 4.28. Concentration of the fourth dissolved chemical at various times for the example of 1-D river/stream flow and transport.

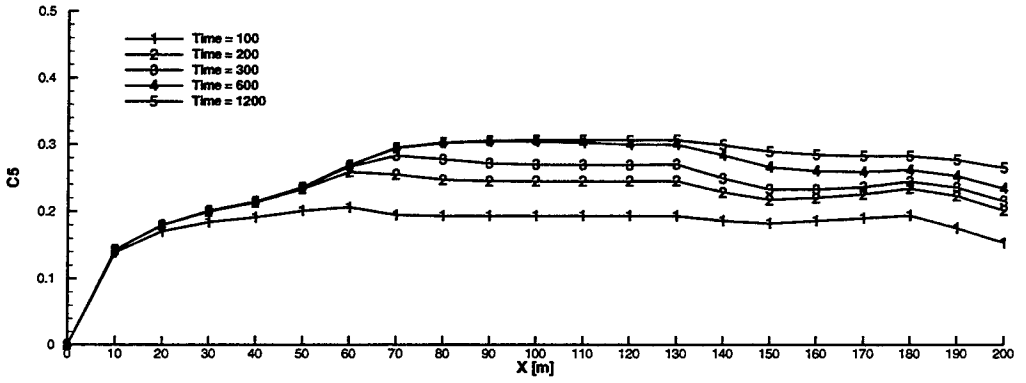


Figure 4.29. Concentration of the fifth dissolved chemical at various times for the example of 1-D river/stream flow and transport.

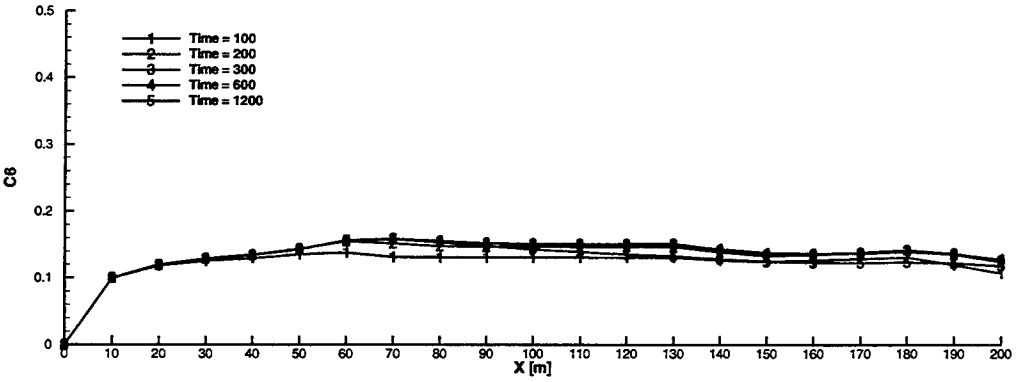


Figure 4.30. Concentration of the sixth dissolved chemical at various times for the example of 1-D river/stream flow and transport.

4.6. Example of 2-D overland flow and transport

The setup for the flow simulation in this example is the same as that in the example of 2-D flow (Section 4.2) except that time step size is 2.5 s for this example. The same chemical system as described in both Sections 4.4 and 4.5 is also considered here. Initially, it is dry and there is no chemical in the domain of interest. As the simulations starts, Dirichlet boundary conditions are applied on the upstream boundary (i.e., X = 0 m) for the transport simulation, where the concentrations of $\overline{C1}$, $\overline{C2}$, $\overline{C3}$ are maintained at 1 g/m^3 and those of $\overline{C4}$, $\overline{C5}$, $\overline{C6}$ are at 0 g/m^3.

Figures 4.31 through 4.37 plot the numerical results at various times. Figure 4.31 is actually representing the same computational result as Figure 4.10 for Example 1 of 2-D overland flow in Section 4.2.1. This is again because this example has a simulation setup identical to that of the example in Section 4.2.1 and the feedback from transport to flow is not considered in the model. Although the results shown in Figures 4.32 through 4.37 are difficult to analyze, we can observe the same concentration distribution trends from upstream to downstream for the six dissolved chemicals as those shown in Figures 4.25 through 4.30. Additionally, it is consistent that $\overline{C3}$ and $\overline{C6}$ are the chemicals having the smallest concentration among the three reactant chemicals and the three product chemicals, respectively, in the downstream region.

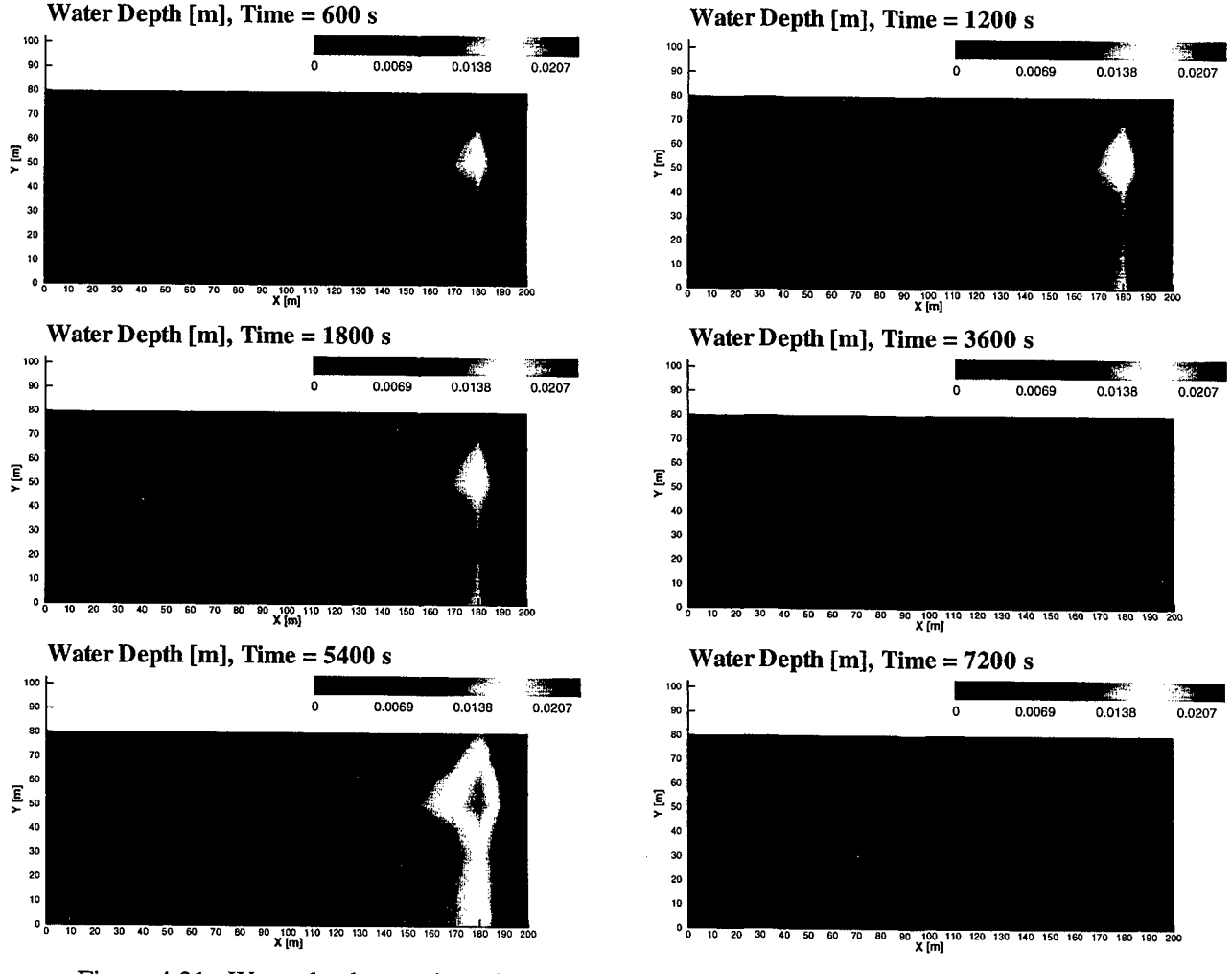


Figure 4.31. Water depth at various times for the example of 2-D overland flow and transport.

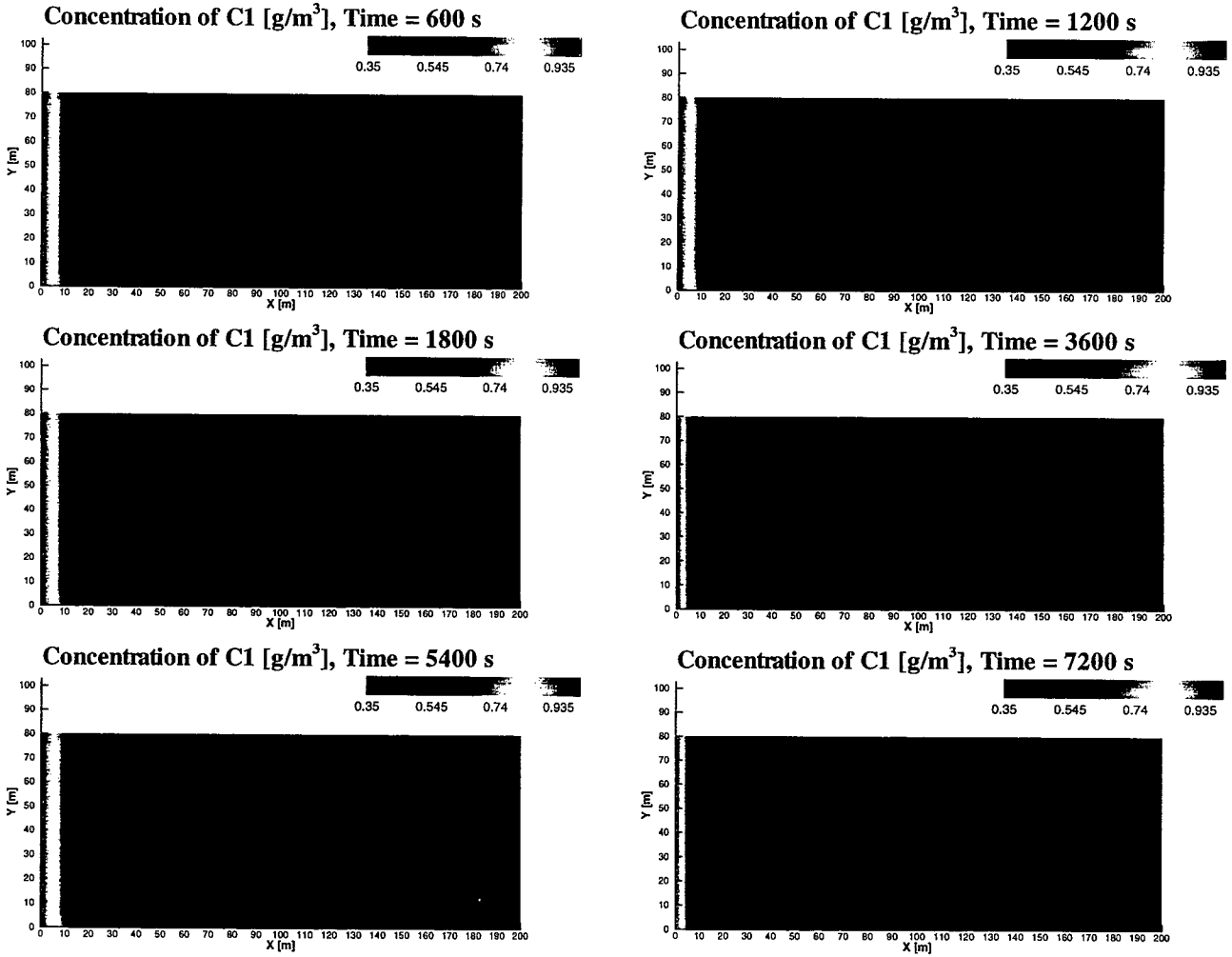


Figure 4.32. Concentration of the first dissolved chemical at various times for the example of 2-D overland flow and transport.

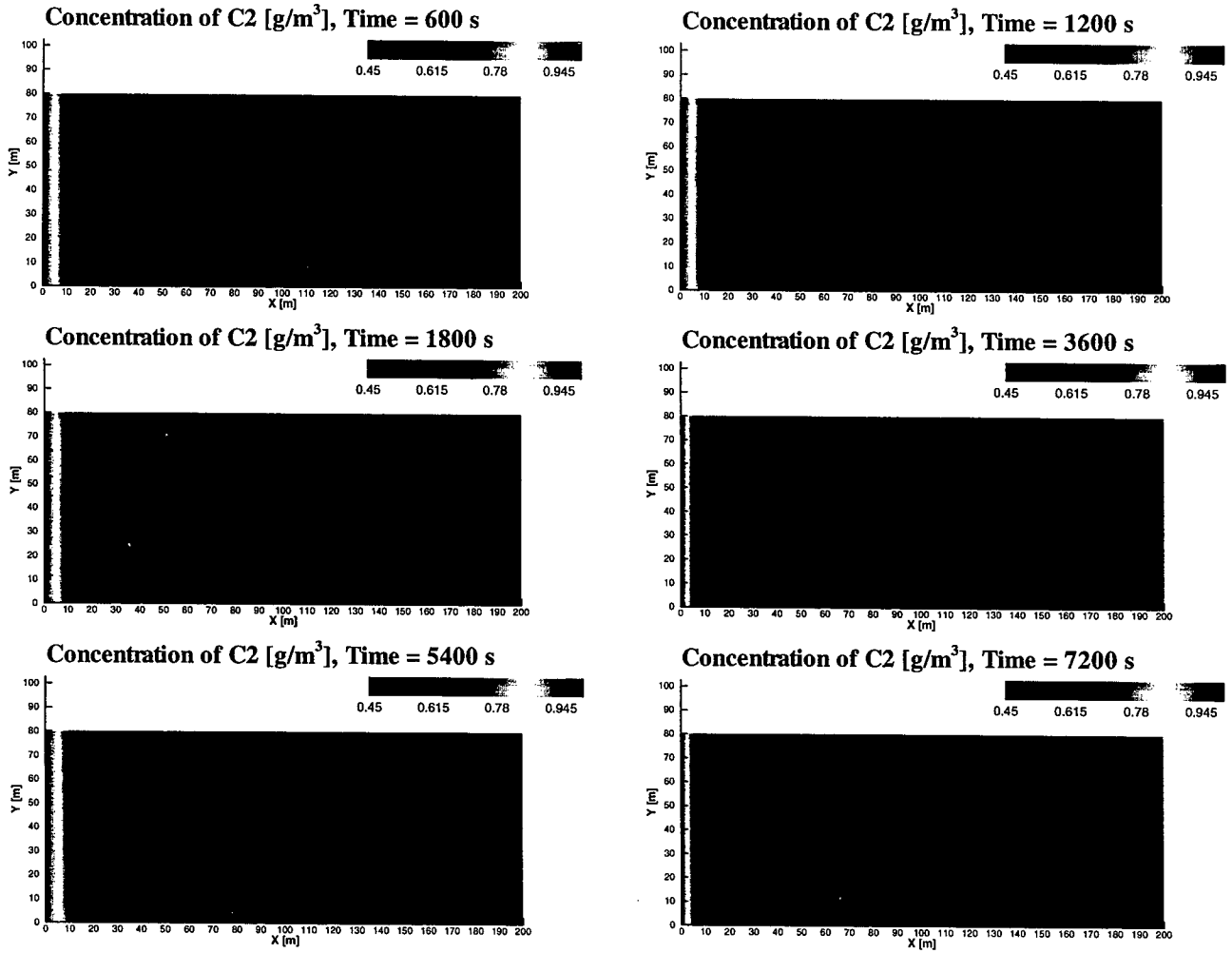


Figure 4.33. Concentration of the second dissolved chemical at various times for the example of 2-D overland flow and transport.

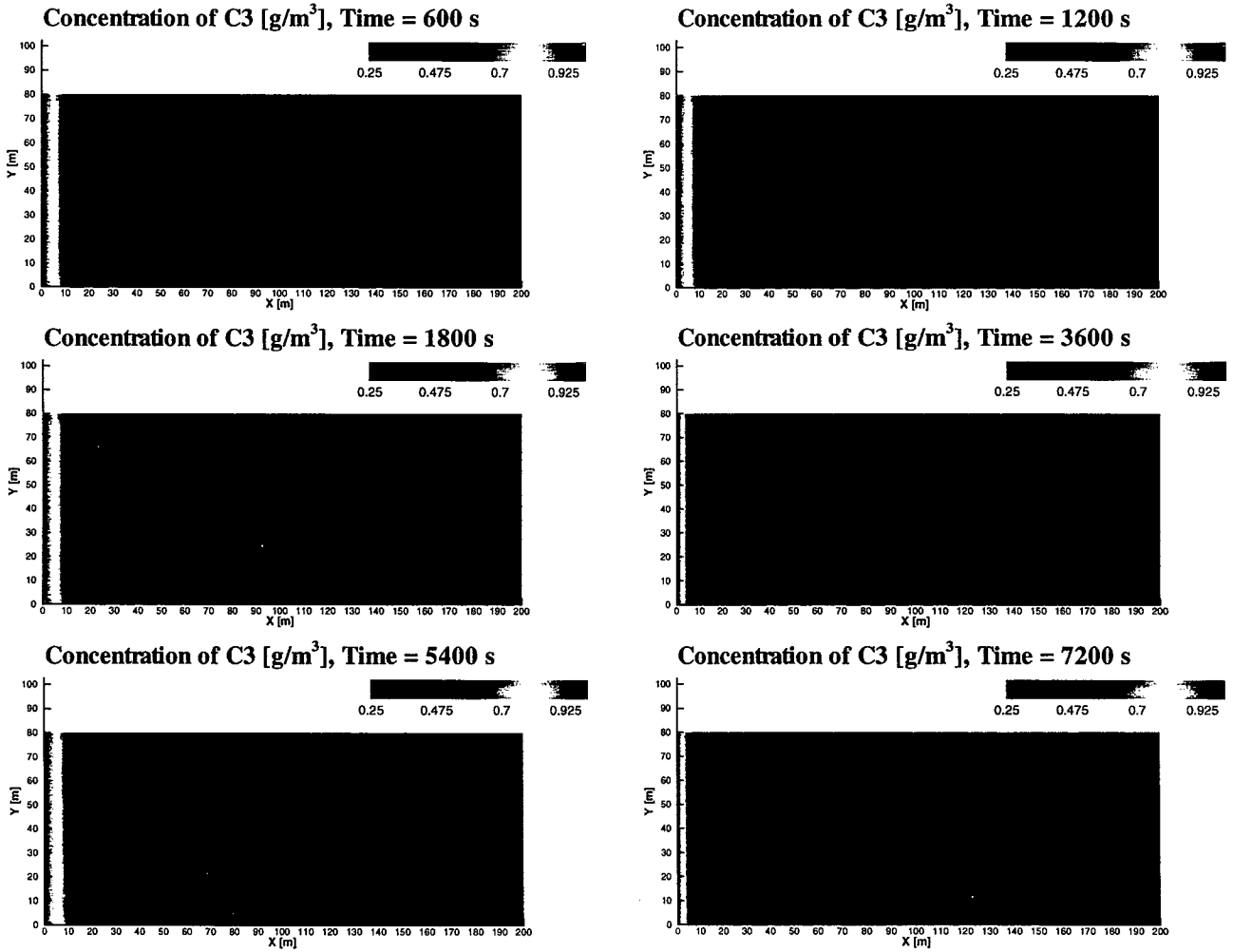


Figure 4.34. Concentration of the third dissolved chemical at various times for the example of 2-D overland flow and transport.

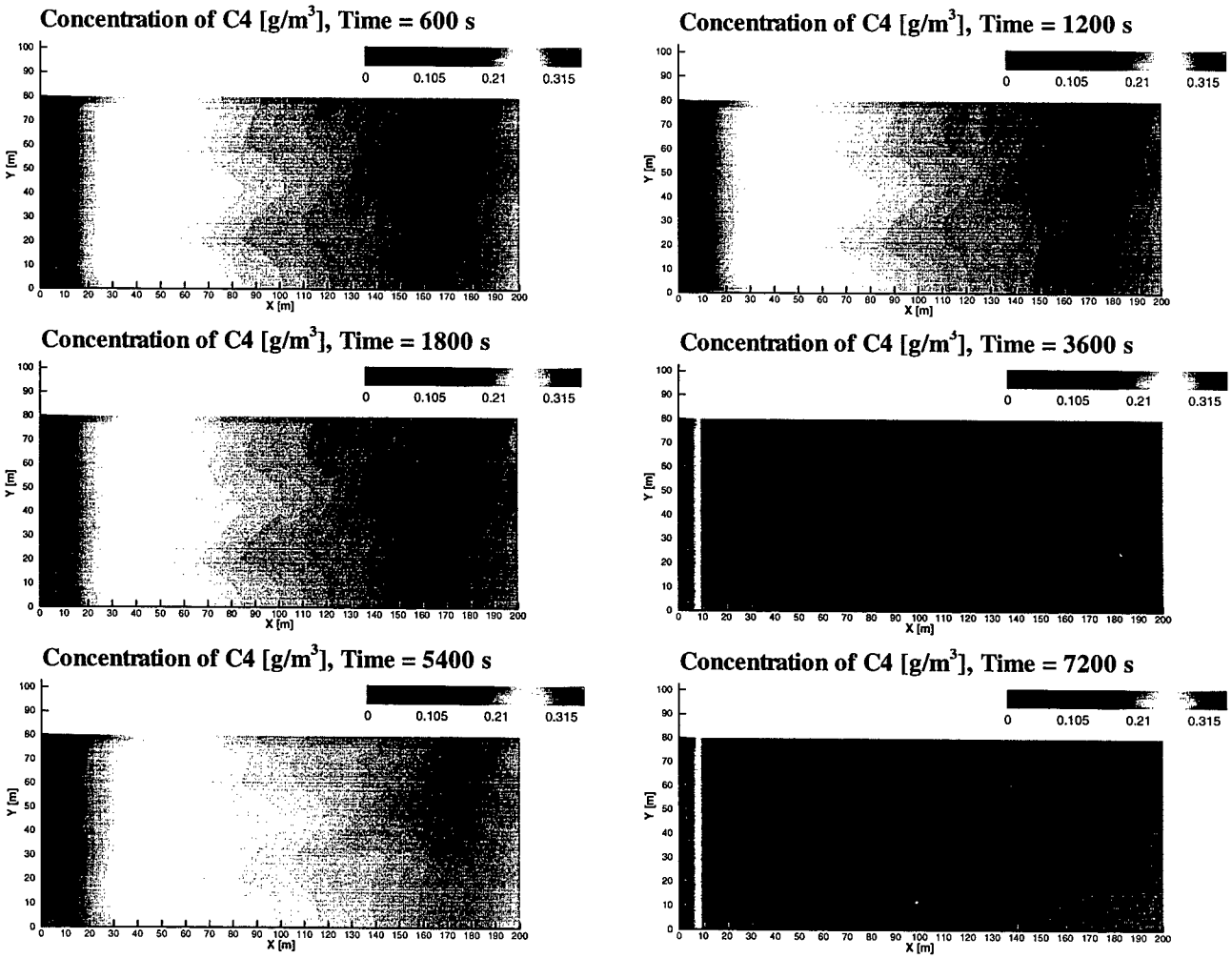


Figure 4.35. Concentration of the fourth dissolved chemical at various times for the example of 2-D overland flow and transport.

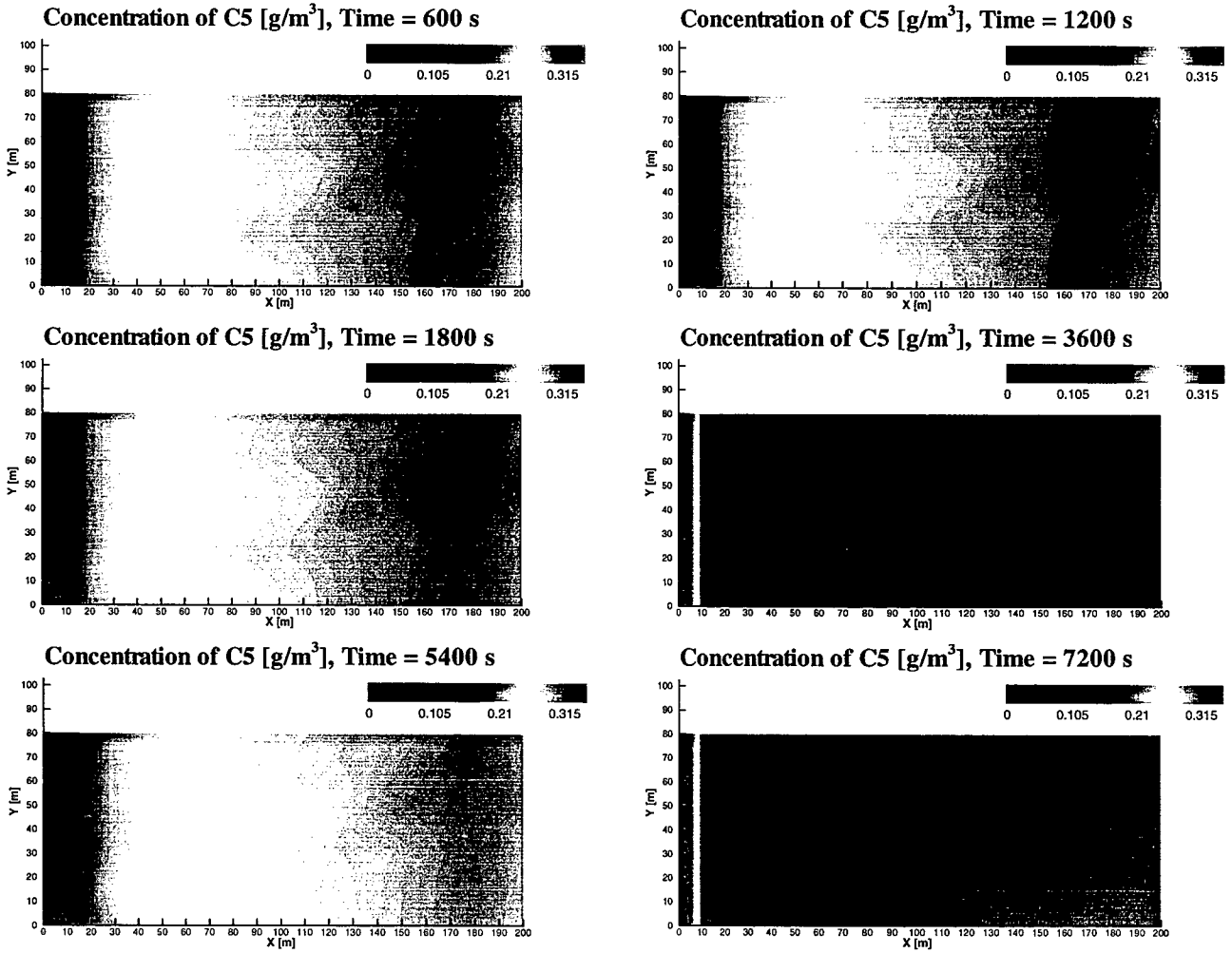


Figure 4.36. Concentration of the fifth dissolved chemical at various times for the example of 2-D overland flow and transport.

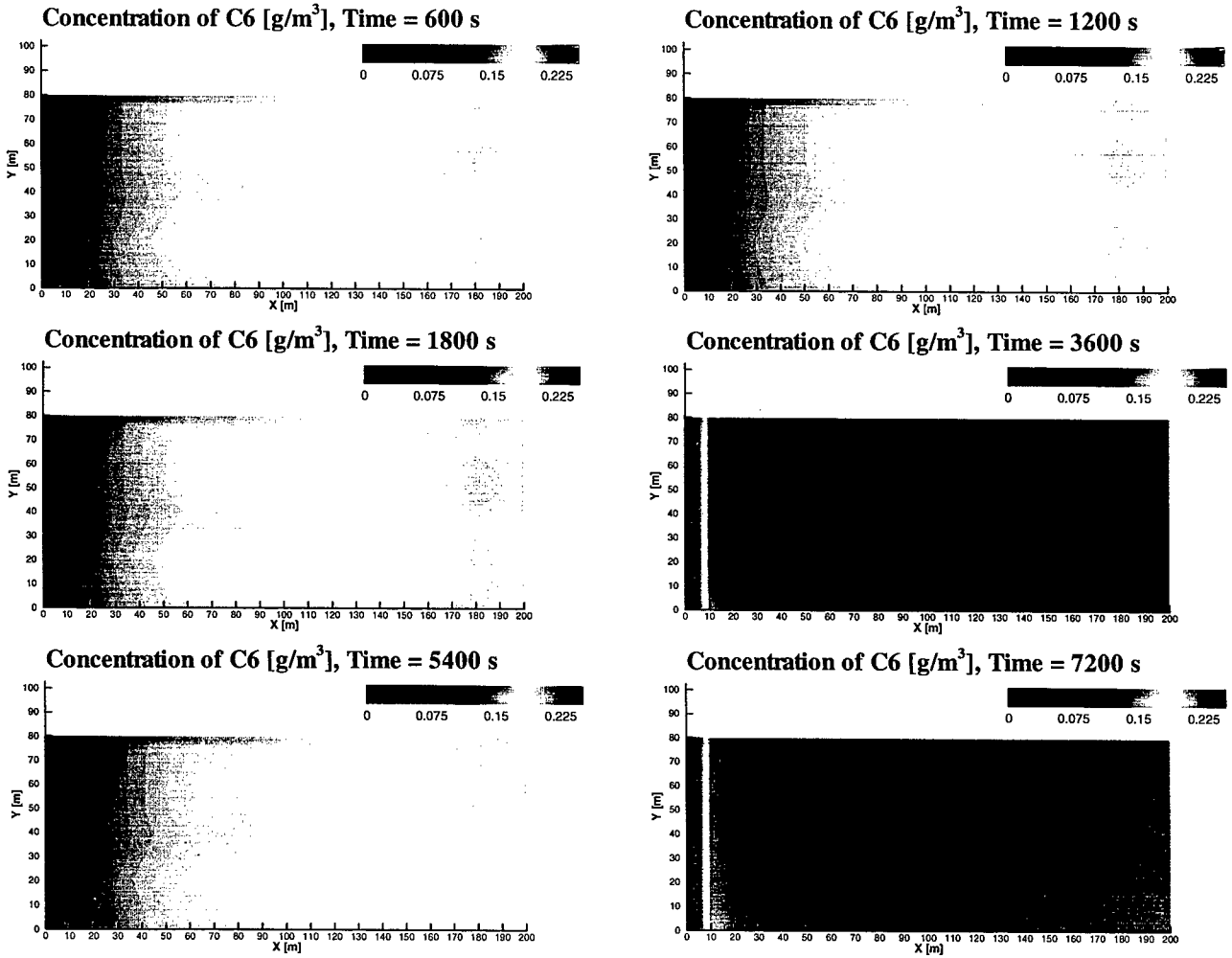


Figure 4.37. Concentration of the sixth dissolved chemical at various times for the example of 2-D overland flow and transport.

4.7. Example of 1-D/2-D flow

A flow system including both 1-D river/stream and 2-D overland is considered in this section. The topography and discretization of the system is plotted in Figure 4.38. As shown in the figure, water would flow from overland into the river/stream that is located in the middle of the system (i.e., the blue strip) and then leave the system through the downstream outlet of the river/stream (i.e., at X = 0 m, Y = 0 m). The slope of river/stream bottom elevation is 0.02.

The river/stream width increases along river/stream's downstream direction: 10 m at Y = 100 and 90 m, 12 m at Y = 80 and 70 m, 14 m at Y = 60 and 50 m, 16 m at Y = 40 and 30 m, 18 m at Y = 20 and 10 m, and 20 m at the outlet (i.e., Y = 0 m). The width changes linearly between any two consecutive locations mentioned above. The system is initially dry. A variable rainfall is applied to the system during a two-hour simulation, which is $5x10^{-7}$ m/s during the first twenty minutes, $1x10^{-6}$ m/s between 20 and 40 minutes, $2x10^{-6}$ m/s between 40 and 60 minutes, no rainfall between 60 and 80 minutes, $4x10^{-6}$ m/s between 80 and 100 minutes, and $5x10^{-7}$ m/s for the last twenty minutes of the simulation. A constant water depth of 0 m is set at the ridge top of the system during the simulation. A water depth-dependent flux boundary condition is employed on the interface between 2-D overland and 1-D river/stream to determine the injection of water from overland to river/stream. Impermeable boundary condition is employed for the overland boundary at Y = 0 m (X = -400 to -10 m and X = 10 to 400 m). The upstream end of the river/stream is treated as a junction, where water budget is used to determine the water depth there. A water depth-dependent flow rate boundary condition is used to compute the water going out from the river/stream downstream boundary, which is also the only outlet of the system. The time step size for 2-D overland flow computation is 20 seconds and it is 2 seconds for calculating 1-D river/stream flow (i.e., 1 2-D time step = 10 1-D time steps).

Figures 4.39 and 4.40 plot water depth and velocity, respectively, at various times for 1-D river/stream. Figure 4.41 depicts the contour of water depth at various times for 2-D overland. From Figure 4.39, we can easily observe the back water effect due to the depth-dependent flow rate at the outlet of 1-D river/stream. Also, we see that the junction (at X = 0 m in Figures 3.39 and 3.40) collects water from the converging overland flow and has the largest water depth in the river/stream. This seems contradictory to our intuition. However, such a result is the consequence of the widening of river width from upstream to downstream and a relatively flat river bottom. Figure 4.41 illustrates how water depth changes with rainfall rates in the overland domain. We can also observe the back water effect due to the depth-dependent normal flux given on the river/stream- and junction-related downstream boundary (i.e., the 1-D/2-D interface boundary).

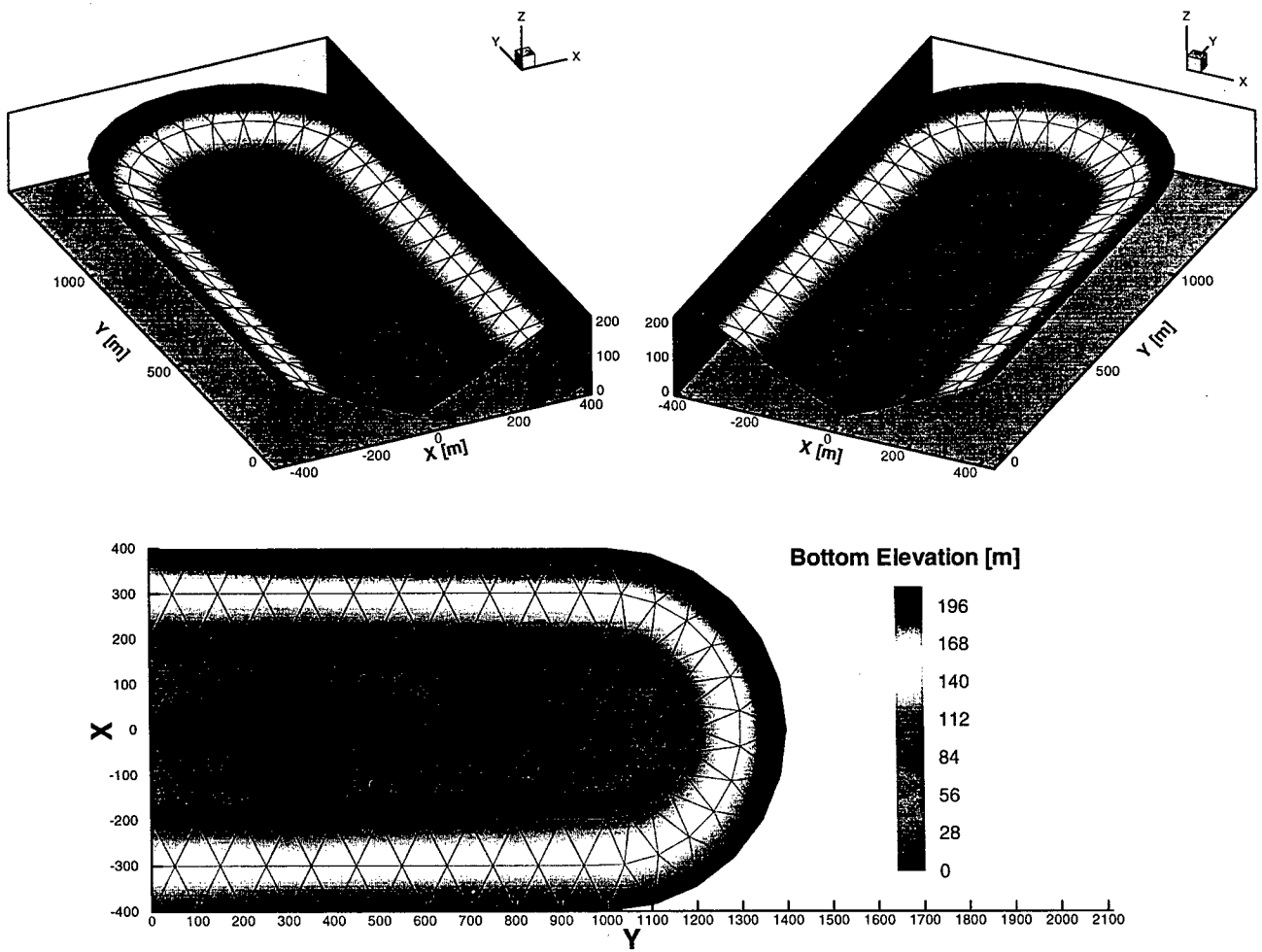


Figure 4.38. The topography and grids for the example of 1-D/2-D flow.

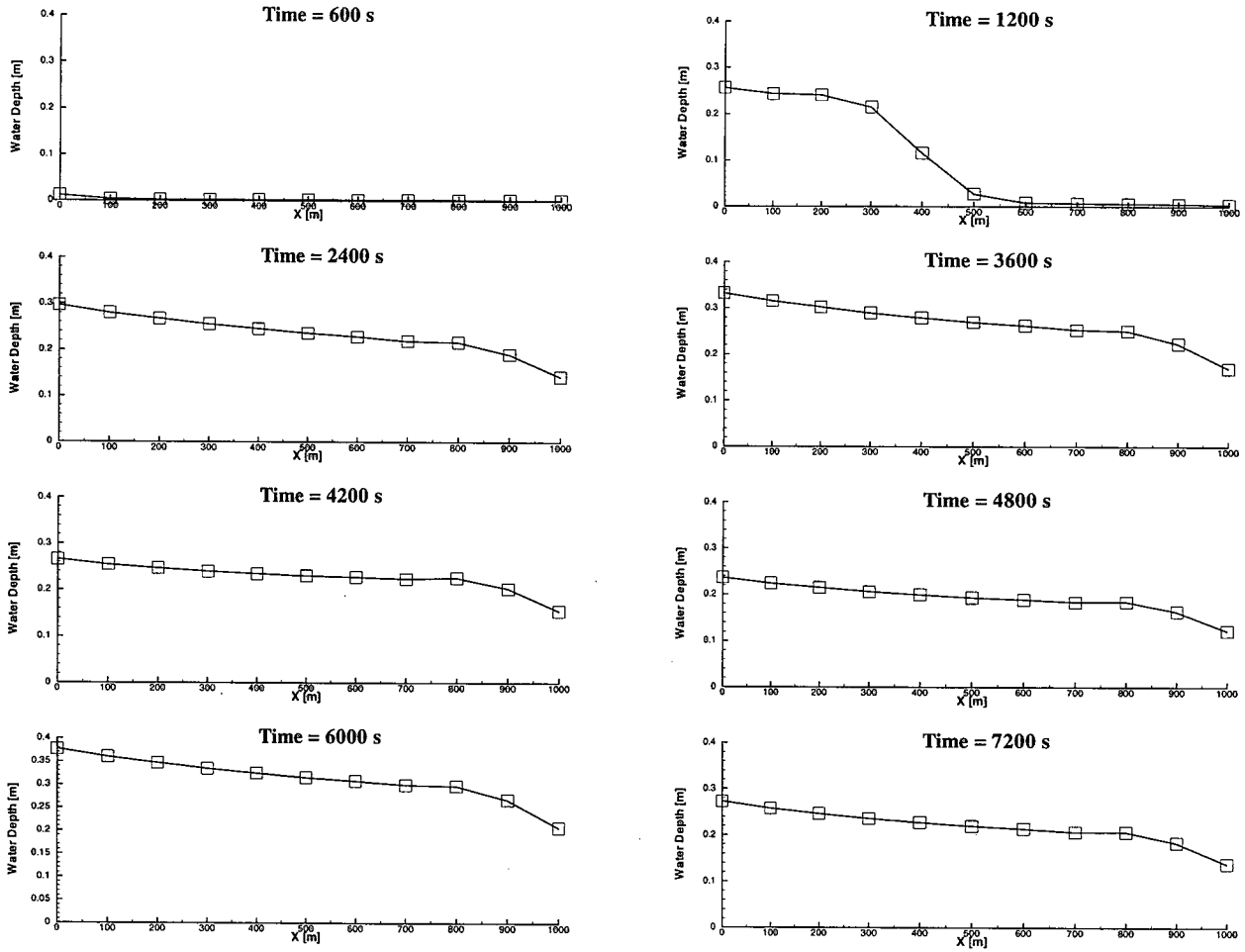


Figure 4.39. Water depth of 1-D river/stream at various times for the example of 1-D/2-D flow.

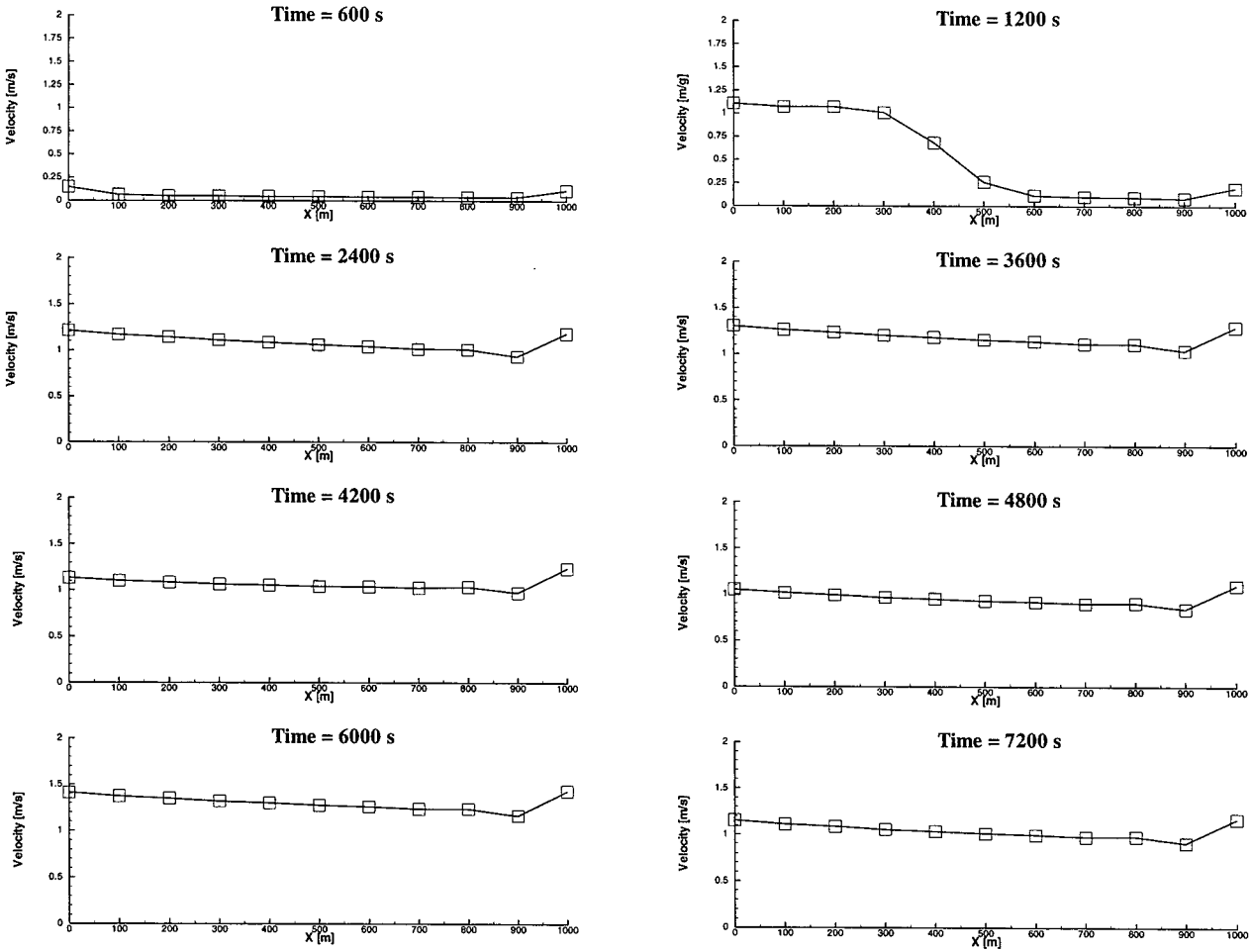


Figure 4.40. Velocity of 1-D river/stream at various times for the example of 1-D/2-D flow.

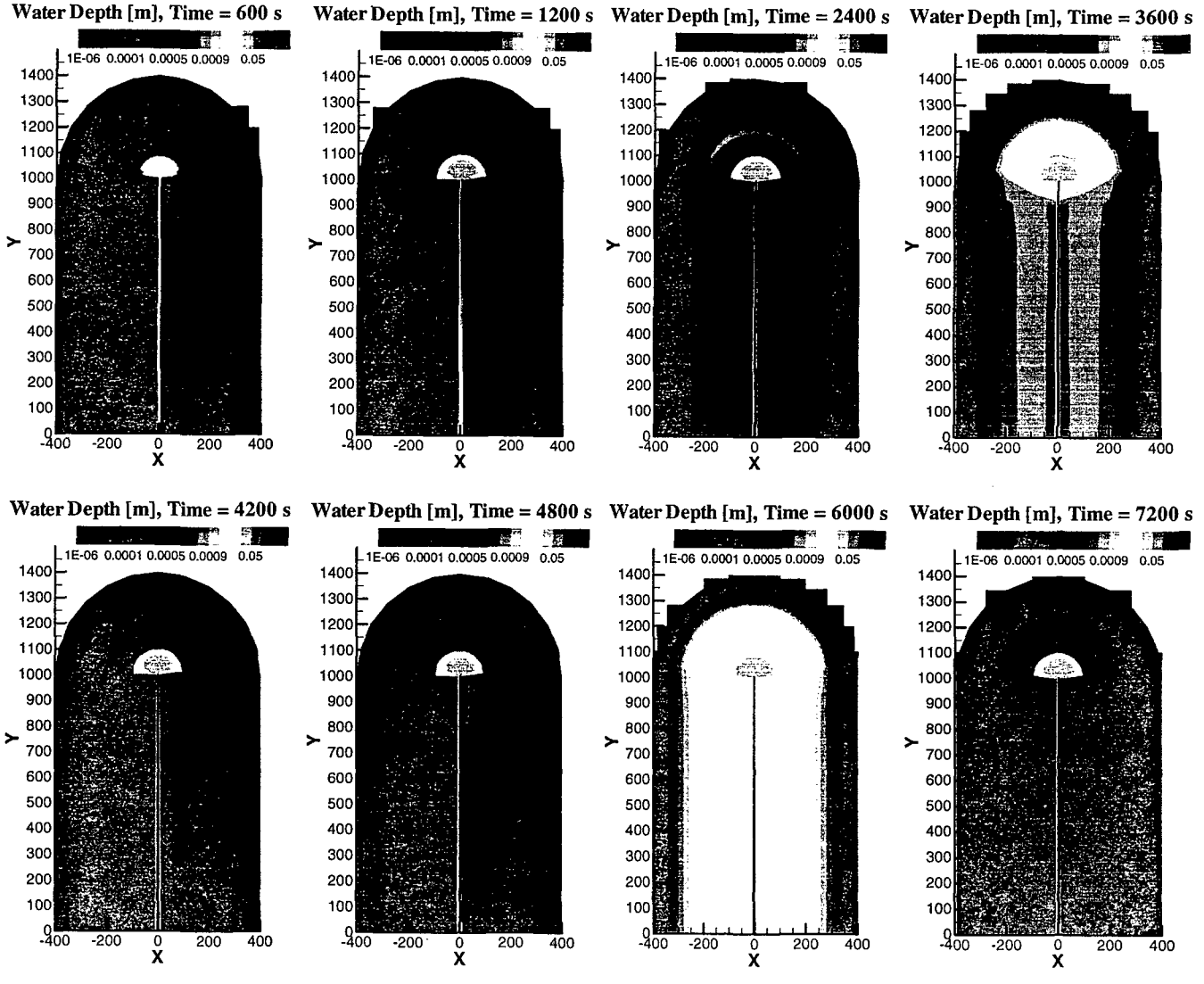


Figure 4.41. Water depth of 2-D overland at various times for the example of 1-D/2-D flow.

4.8. Example of 1-D/2-D flow and transport

This example considers both flow and transport in 1-D river/stream and 2-D overland. The topography and grids are shown in Figure 4.42 where flow is driven into the river/stream from the overland simply due to gravity. The slope of river bottom elevation is 0.01.

The river/stream has a uniform width of 10 m. The system is initially dry. A variable rainfall is applied to the system during a two-hour simulation, which is 10^{-5} m/s during the first twenty minutes, $2x10^{-5}$ m/s between 20 and 40 minutes, 10^{-5} m/s between 40 and 60 minutes, $2x10^{-5}$ m/s between 60 and 80 minutes, 10^{-5} m/s between 80 and 100 minutes, and no rainfall for the last twenty minutes of the simulation. A constant water depth of 10^{-4} m is set at the ridge top of the system during the simulation. A water depth-dependent flux boundary condition is employed on the interface between 2-D overland and 1-D river/stream to determine the injection of water from overland to river/stream. Impermeable boundary condition is employed for the overland boundary at Y = 0 m and Y = 900 m (X = 200 to 595 m and X = 605 to 1000 m). Water depth is maintained at 10^{-3} m at the upstream end of the river/stream. A water depth-dependent flow rate boundary condition is used to compute the water going out from the river/stream downstream boundary. Manning's roughness is 0.01 for overland and 0.03 for river/stream. The time step size for 2-D overland flow computation is 10 seconds and it is 2 seconds for calculating 1-D river/stream flow.

As for the transport simulation, six dissolved chemicals and two reactions are taken into account. Among the six chemicals, five of them are involved in the two reactions as described in the following and the other one is non-reactive.

$$\overline{C1} + \overline{C2} \rightleftharpoons \overline{C4} \qquad k_f = 0.01, \quad k_b = 0.005 \tag{1}$$

$$\overline{C1} + \overline{C3} \rightleftharpoons \overline{C5} \qquad k_f = 0.01, \quad k_b = 0.005 \tag{2}$$

The dissolved chemical $\overline{C5}$ is radioactive and the decay constant is 10^{-4} 1/s. $\overline{C1}$, $\overline{C2}$, $\overline{C3}$, and $\overline{C6}$ exist in rainfall with a constant concentration of 1 g/m^3. In 2-D overland transport, Variable boundary conditions are applied on both the upstream boundary (i.e., ridge top), where the concentration is 1 g/m^3 for $\overline{C1}$, $\overline{C2}$, $\overline{C3}$, and $\overline{C6}$, and is 0 g/m^3 for the other two chemicals if the flow is directed into the domain of interest. For the overland-river interface, we also apply variable boundary conditions by using the respective concentrations in the channel as the incoming concentrations when the flow is directed from river/stream to overland on the interface boundary. As for 1-D river/stream transport, the same variable boundary condition as is employed for the overland ridge top is applied to both the upstream and the downstream boundary nodes (i.e., located at (600 m, 900 m) and (600 m, 0 m), respectively).

Figures 4.43 and 4.44 plot water depth at various times for 1-D river/stream and 2-D overland,

respectively. Figures 4.45 through 4.50 depict the concentration of the first through the sixth dissolved chemicals, respectively, at various times for 1-D transport. Figures 4.51 through 4.56 show the concentration of the first through the sixth dissolved chemicals, respectively, at various times for 2-D overland.

Both Figures 4.43 and 4.44 indicate that steady state have been reached by the end of each constant rainfall period of time (each rainfall period lasts for twenty minutes). For both 1-D and 2-D flows, the back water effect is obvious. The reason has been given in the previous example. Figures 4.50 and 4.56 show the uniformly distributed concentration of the nonreactive dissolved chemical in 1-D and 2-D, respectively. This numerical result help to verify our model when 1-D flow, 2-D flow, 1-D transport, and 2-D transport are all taken into account.

Since the second and the third dissolved chemicals are involved in identical aqueous complexation reactions, they should have the same concentration distribution, so should their respective product chemicals (i.e., the fourth and the fifth chemicals, respectively). However, the radioactive nature of the fifth chemical makes the difference between them as well as the difference between their respect product chemicals. On the other hand, the decay is so slow so that the difference mentioned above is almost invisible (compare Figures 4.46 with 4.47, Figures 4.48 with 4.49, Figures 4.52 with 4.53, and Figures 4.54 with 4.55).

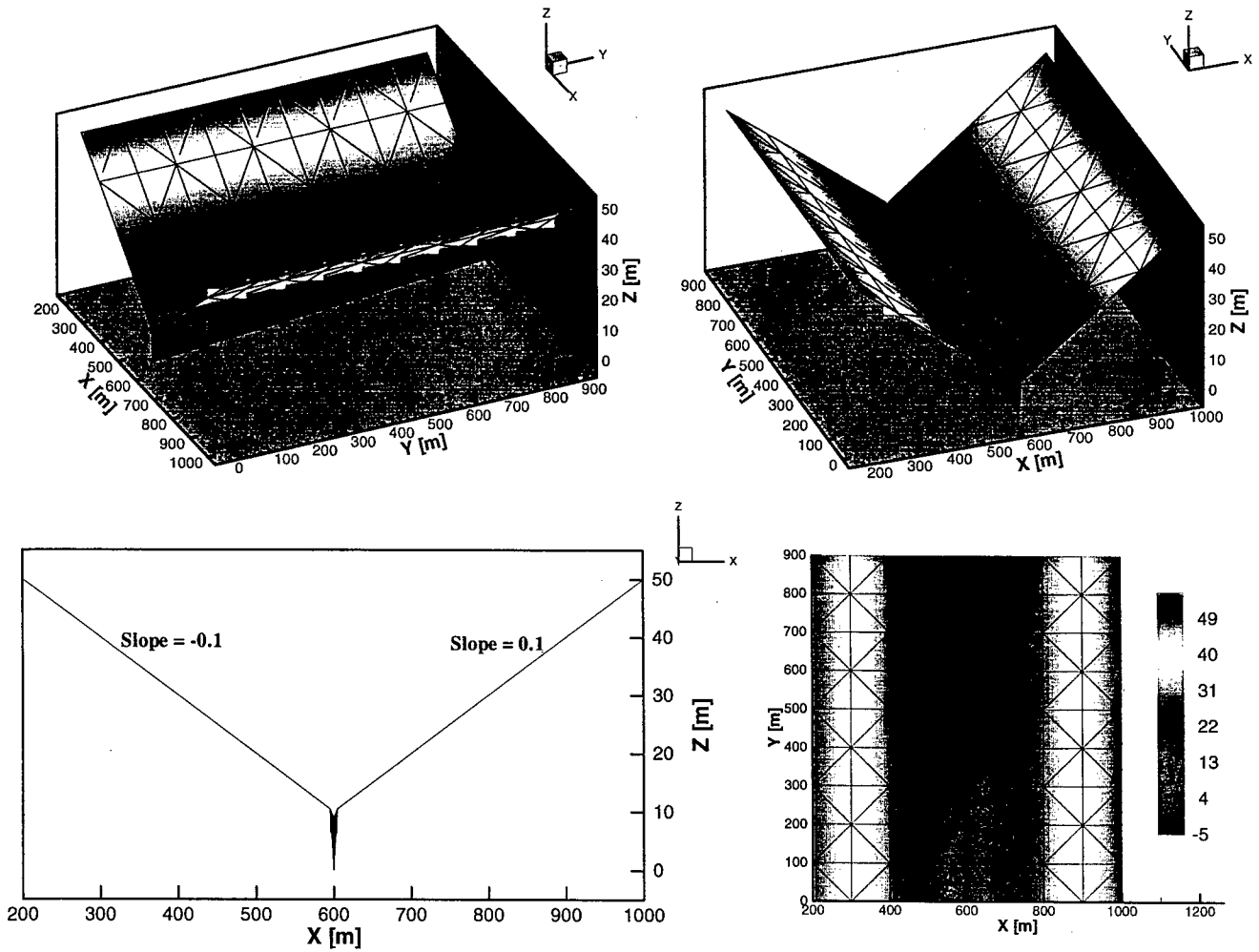


Figure 4.42. The topography and grids for the example of 1-D/2-D flow and transport.

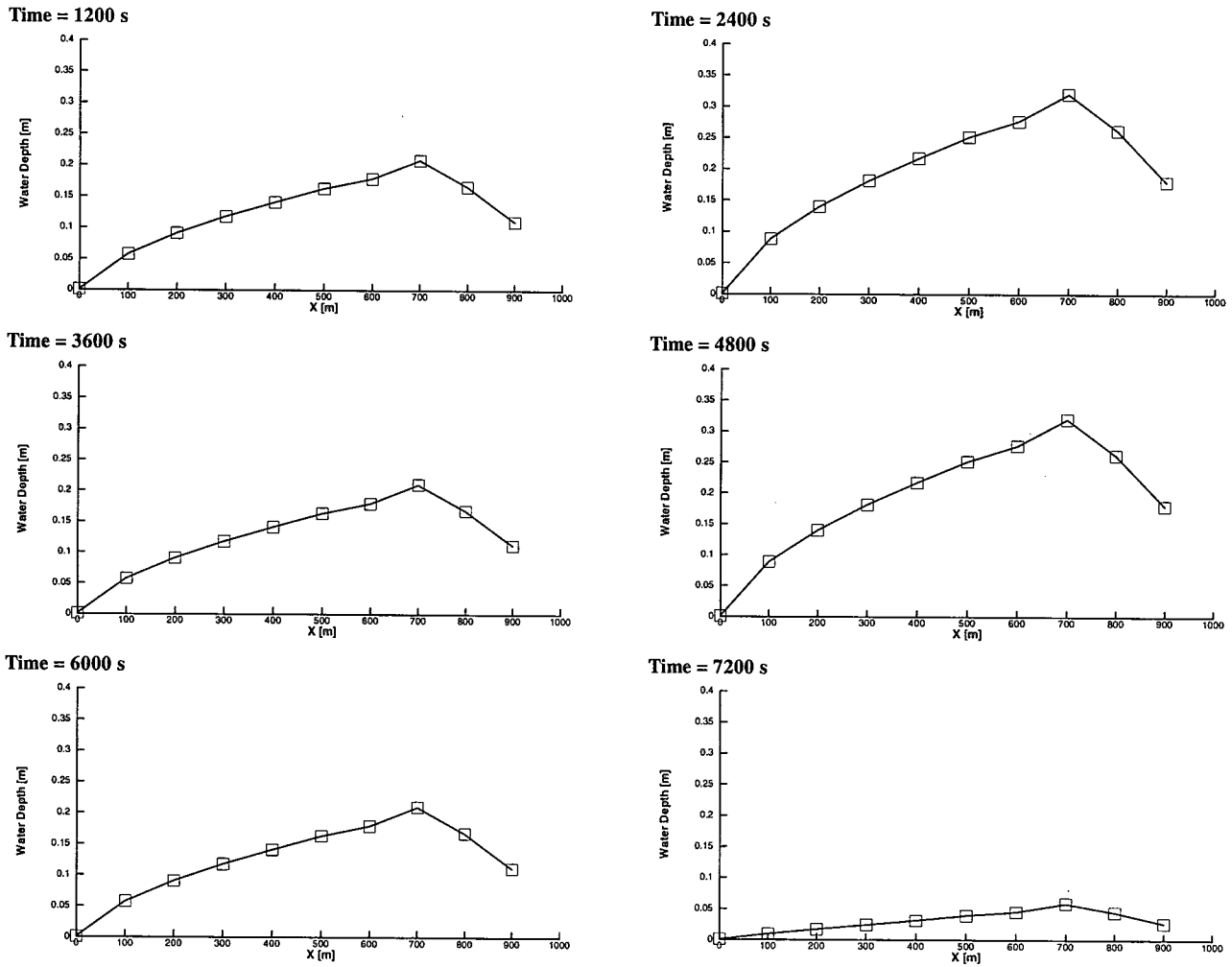


Figure 4.43. Water depth of 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

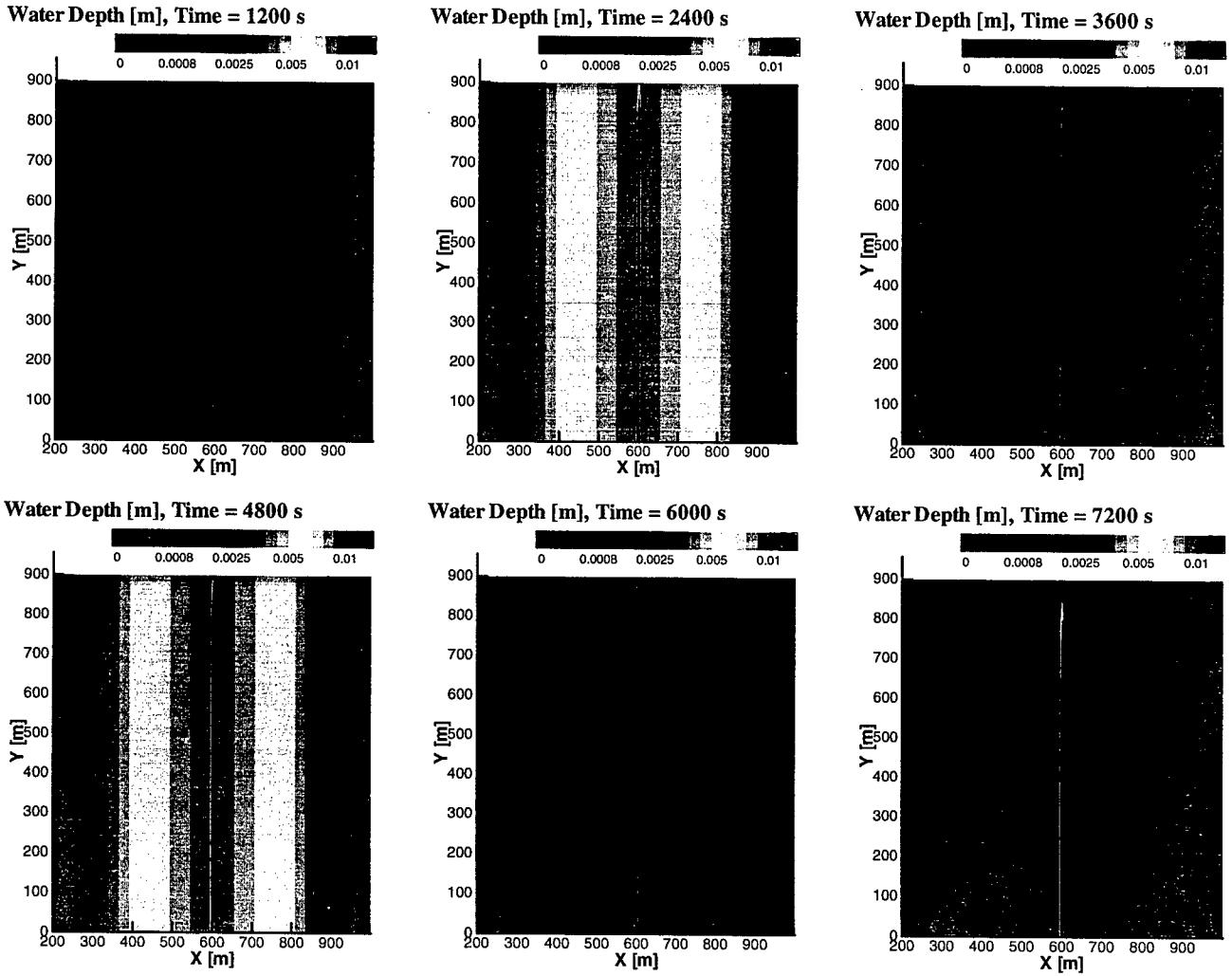


Figure 4.44. Water depth contour of 2-D overland at various times for the example of 1-D/2-D flow and transport.

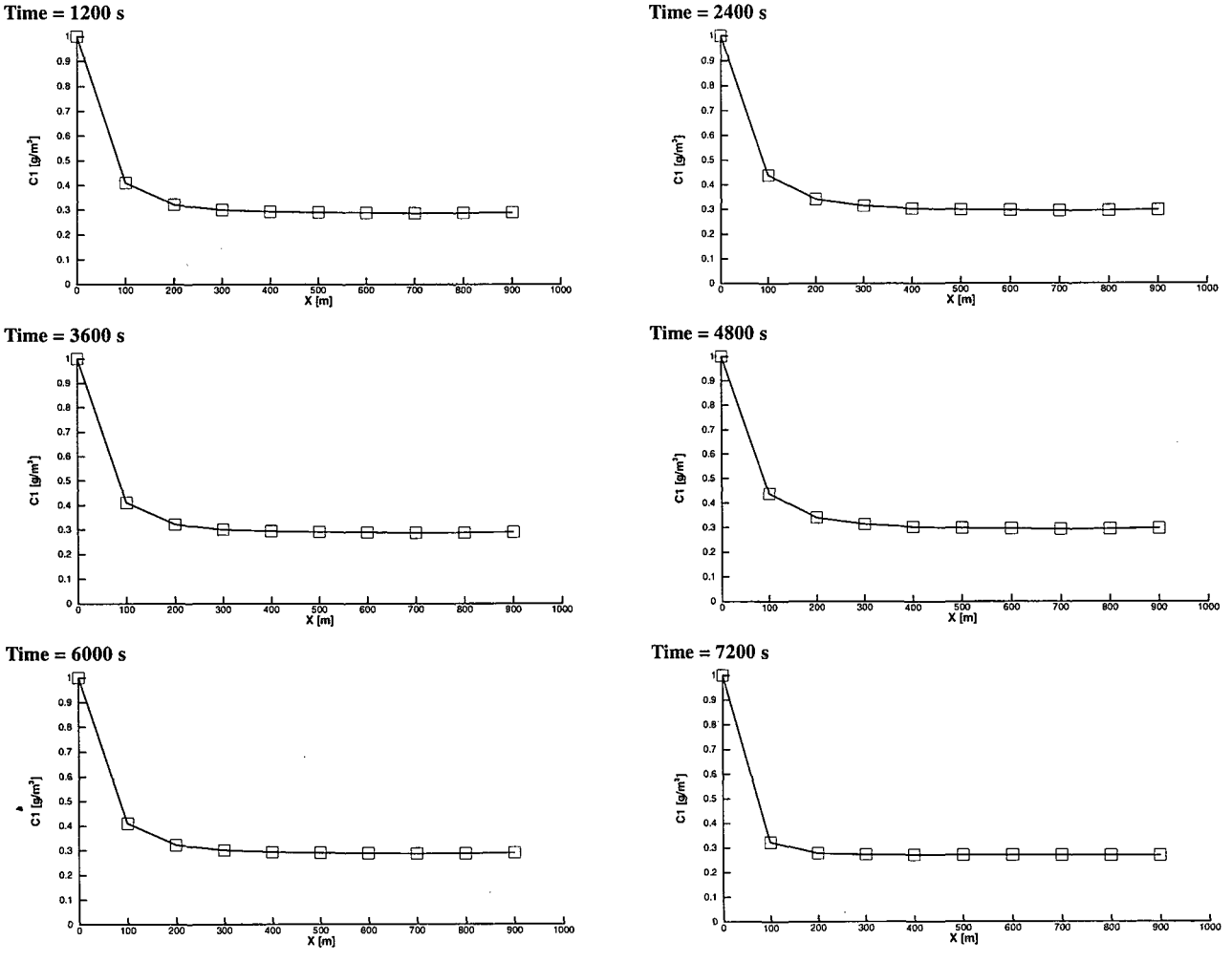


Figure 4.45. Concentration of the first dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

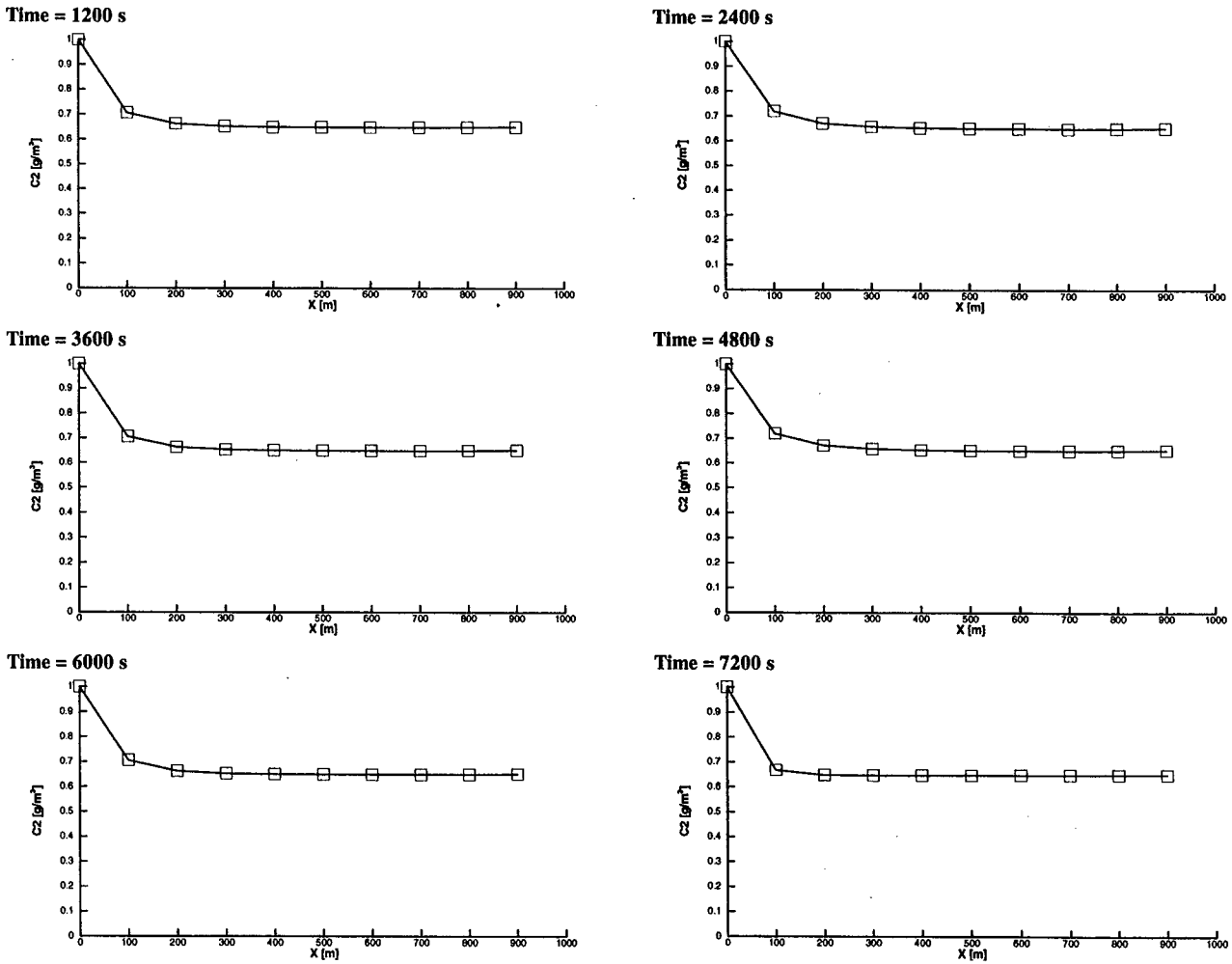


Figure 4.46. Concentration of the second dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

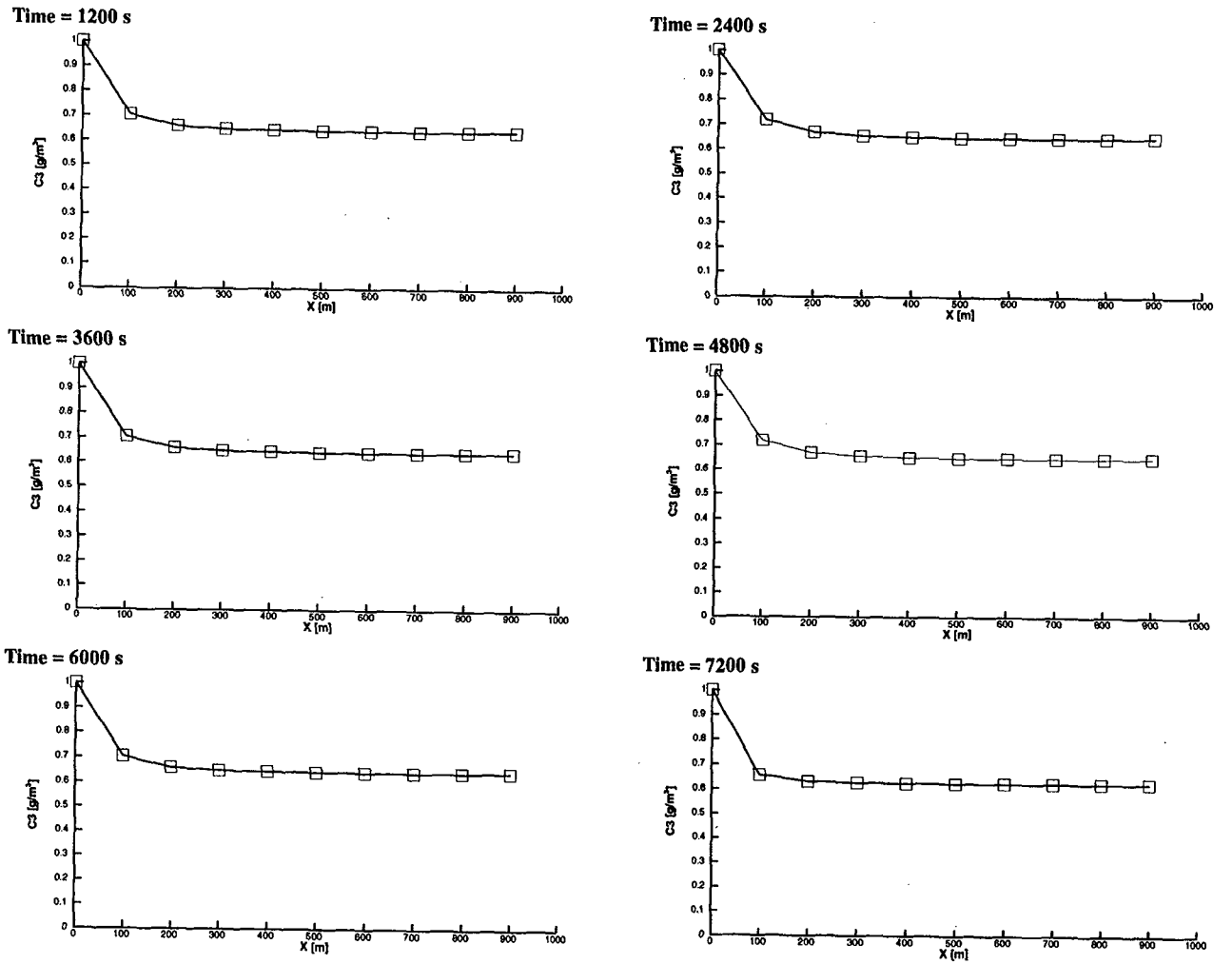


Figure 4.47. Concentration of the third dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

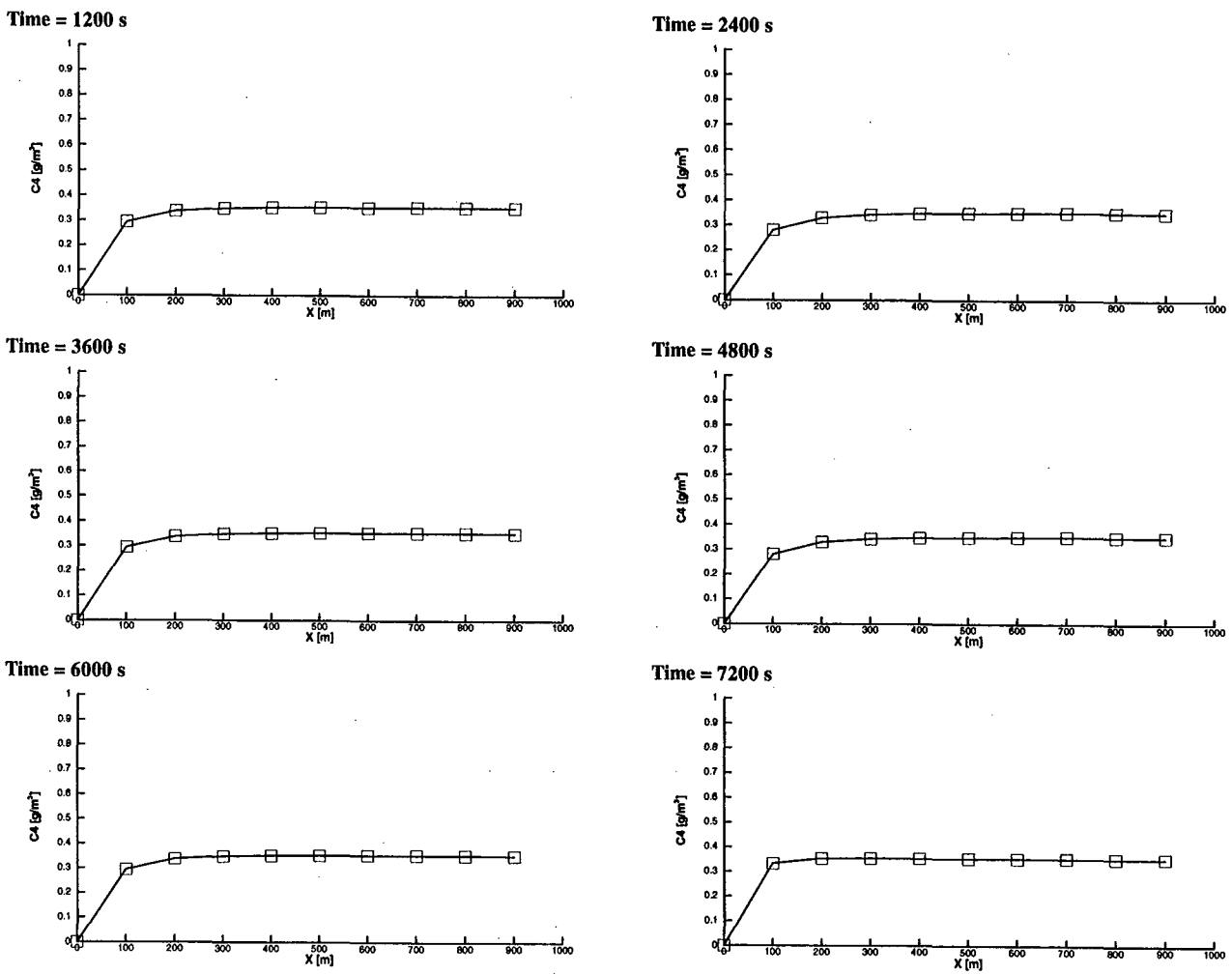


Figure 4.48. Concentration of the fourth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

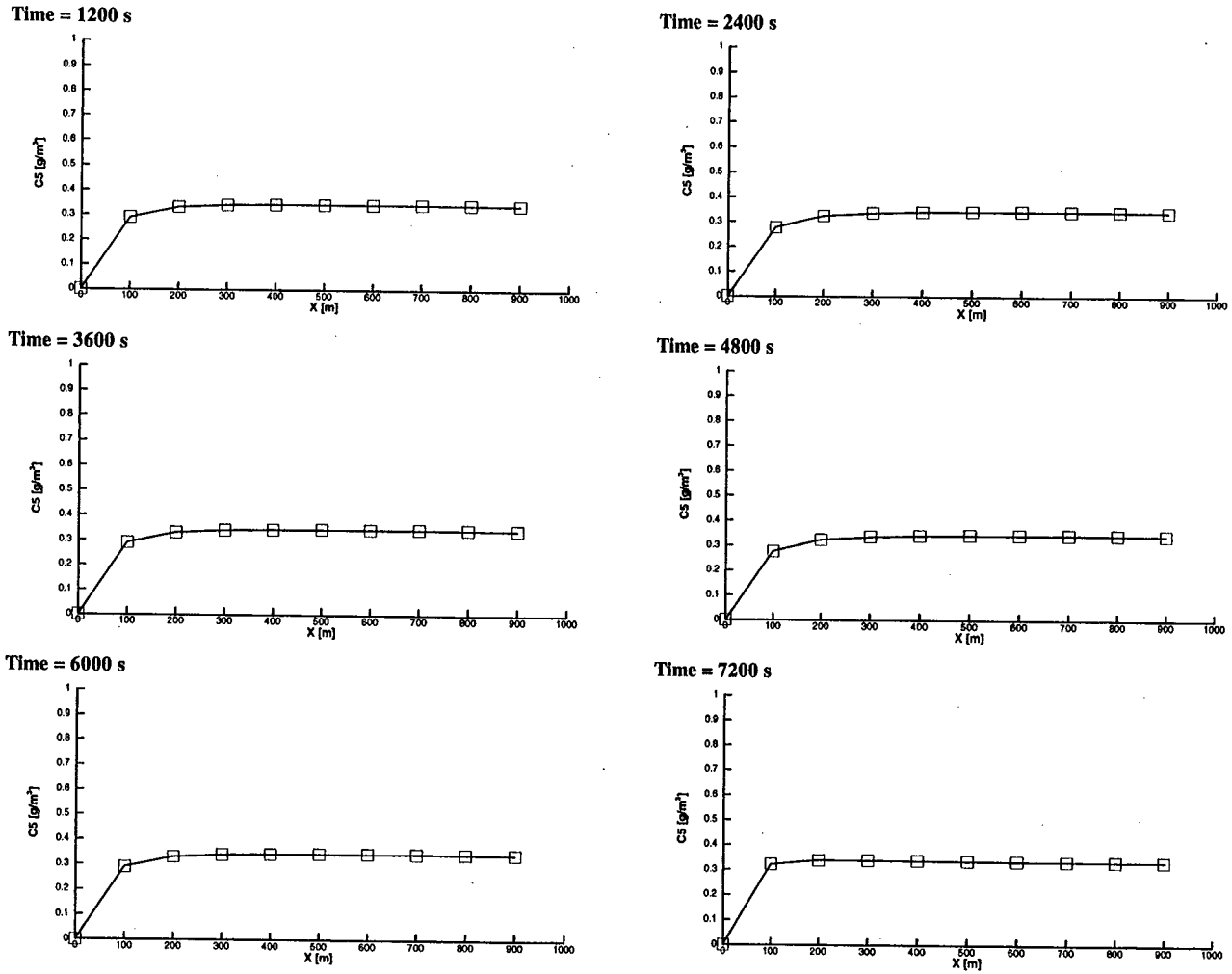


Figure 4.49. Concentration of the fifth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

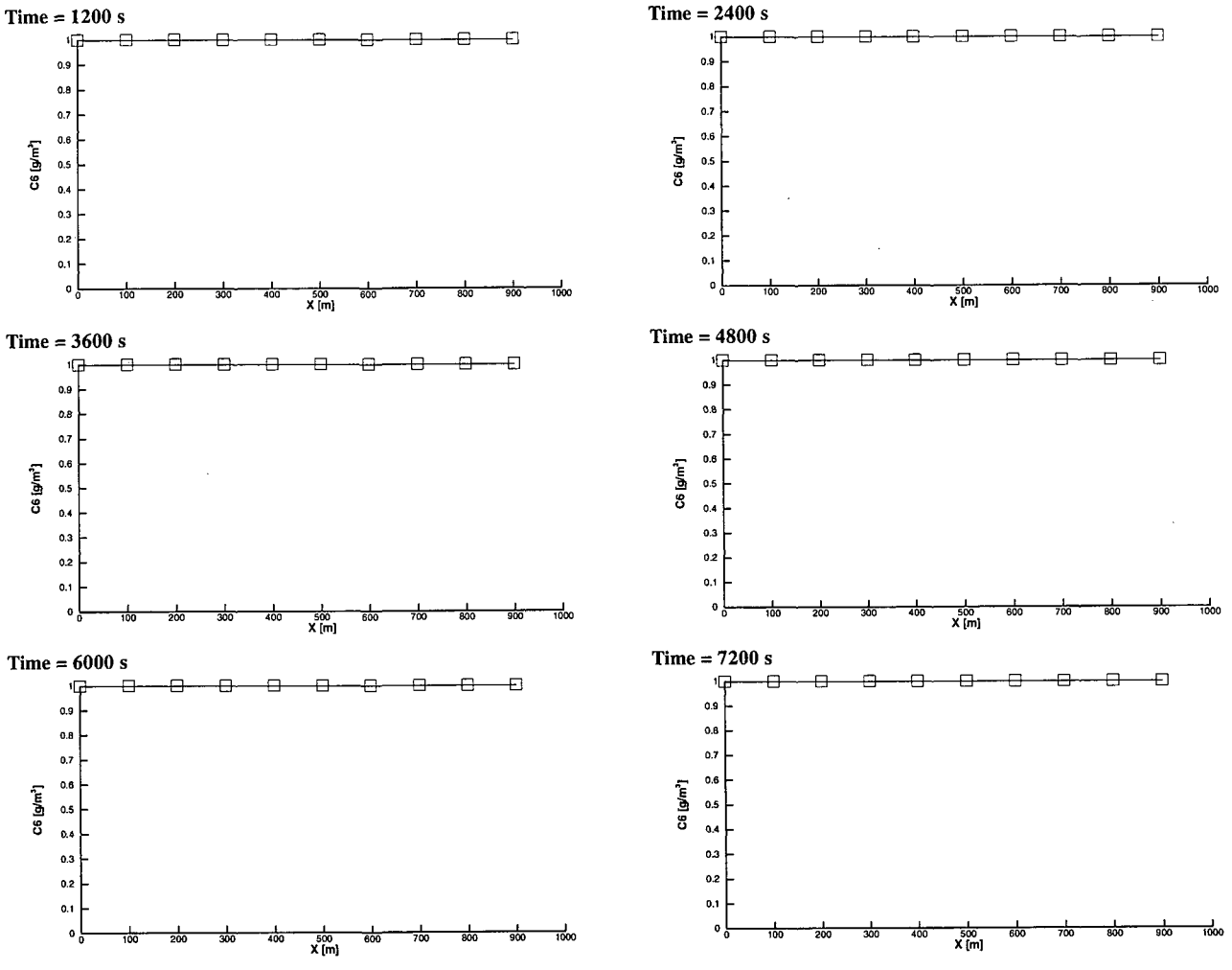


Figure 4.50. Concentration of the sixth dissolved chemical in 1-D river/stream at various times for the example of 1-D/2-D flow and transport.

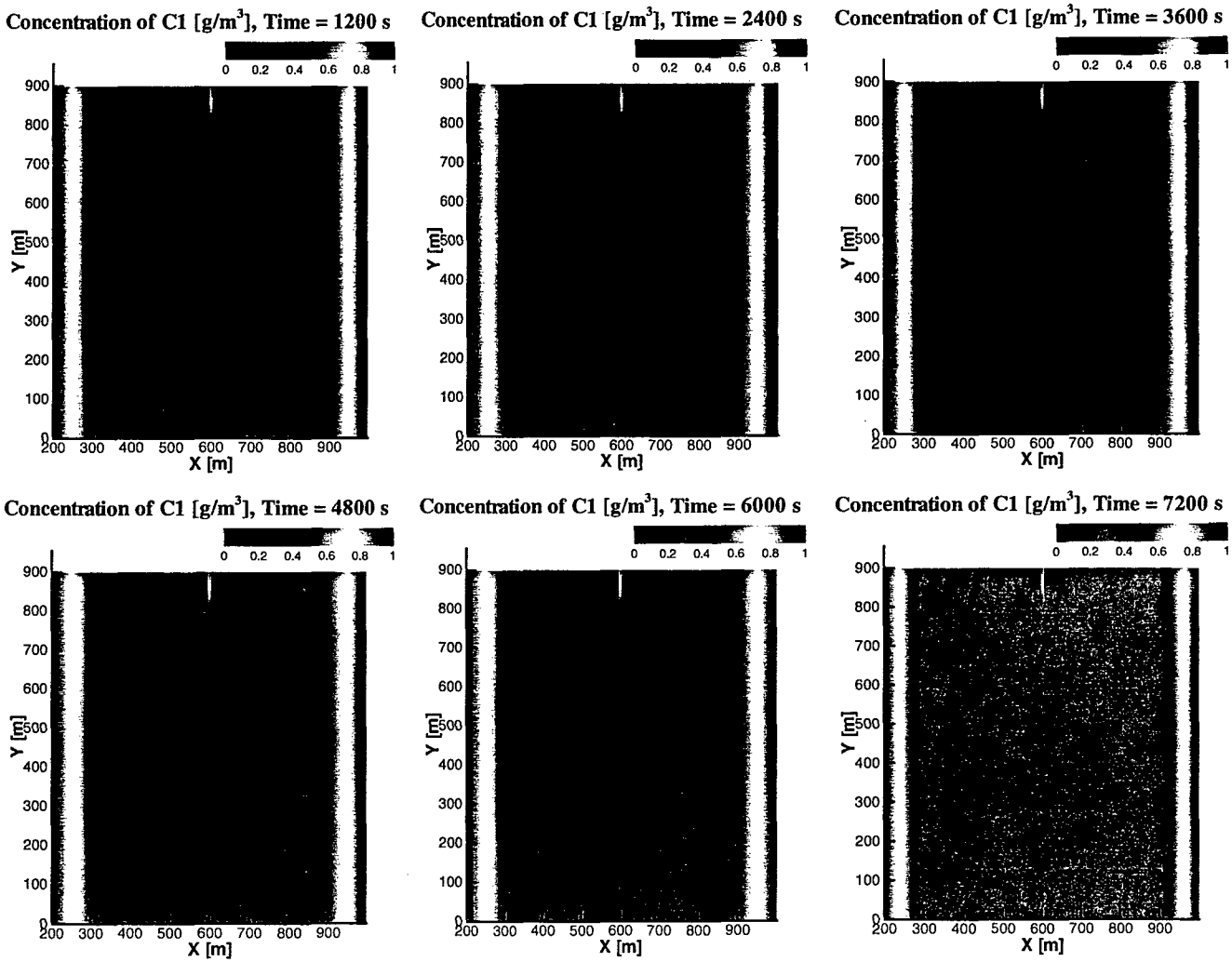


Figure 4.51. Concentration of the first dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport.

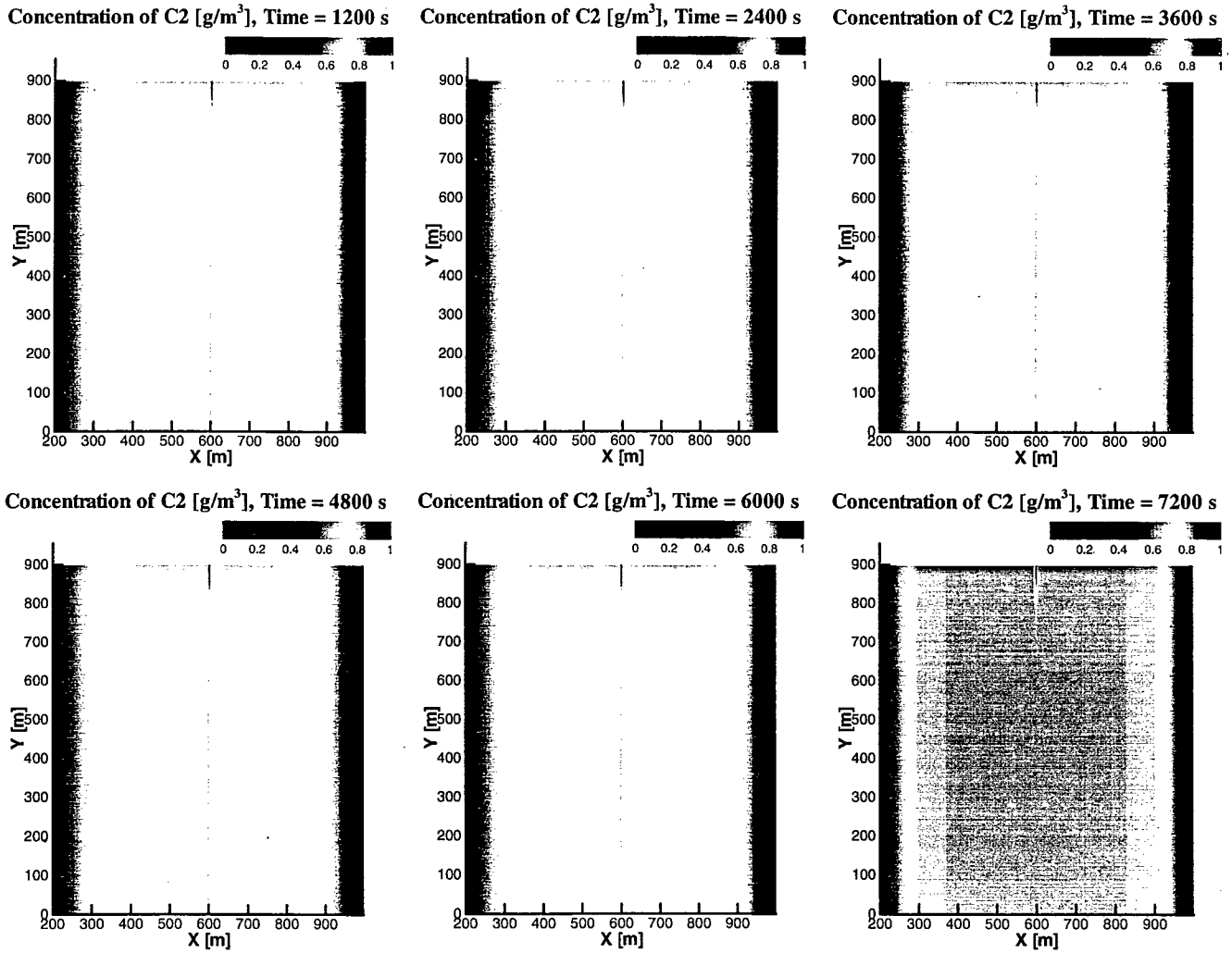


Figure 4.52. Concentration of the second dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport.

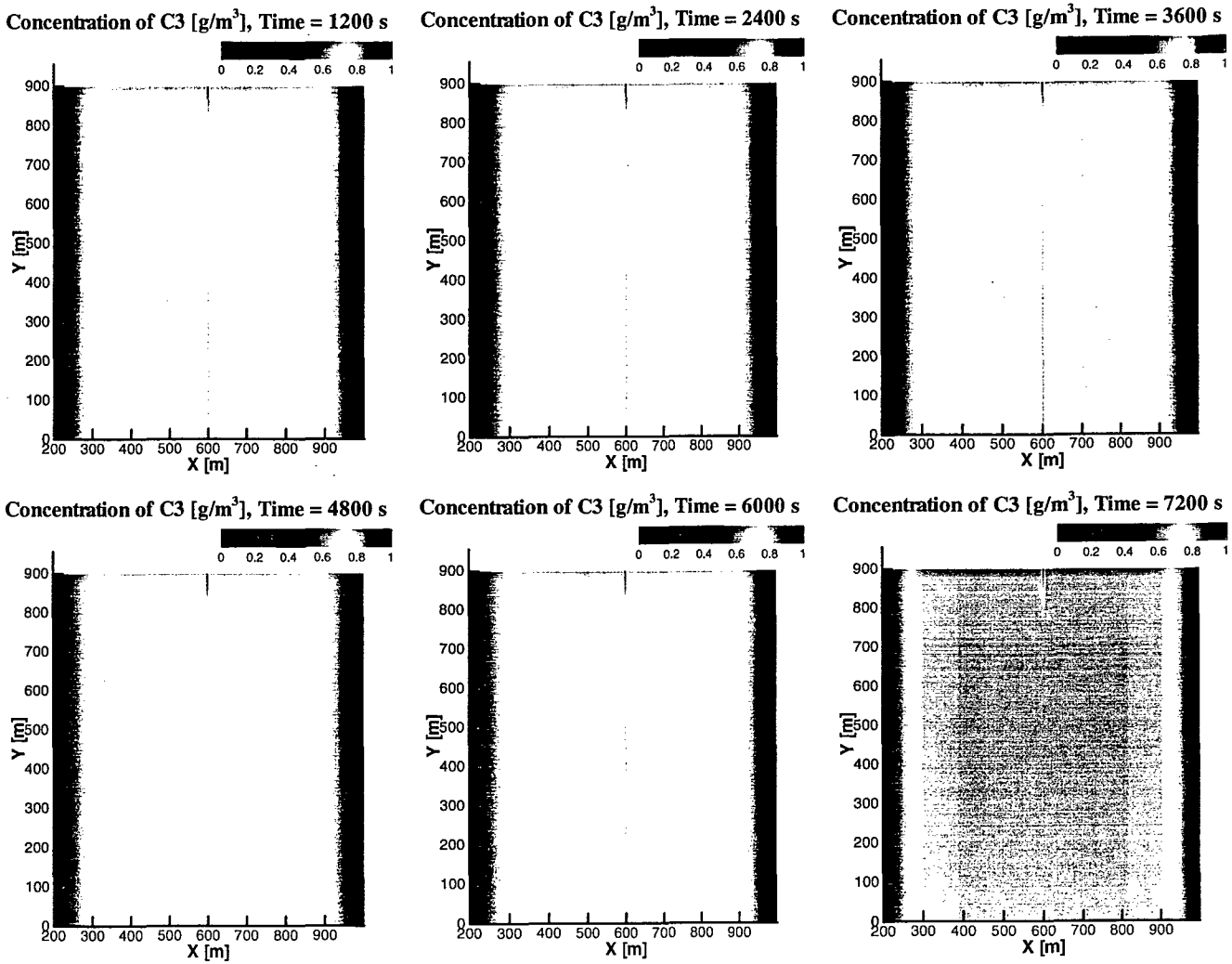


Figure 4.53. Concentration of the third dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport.

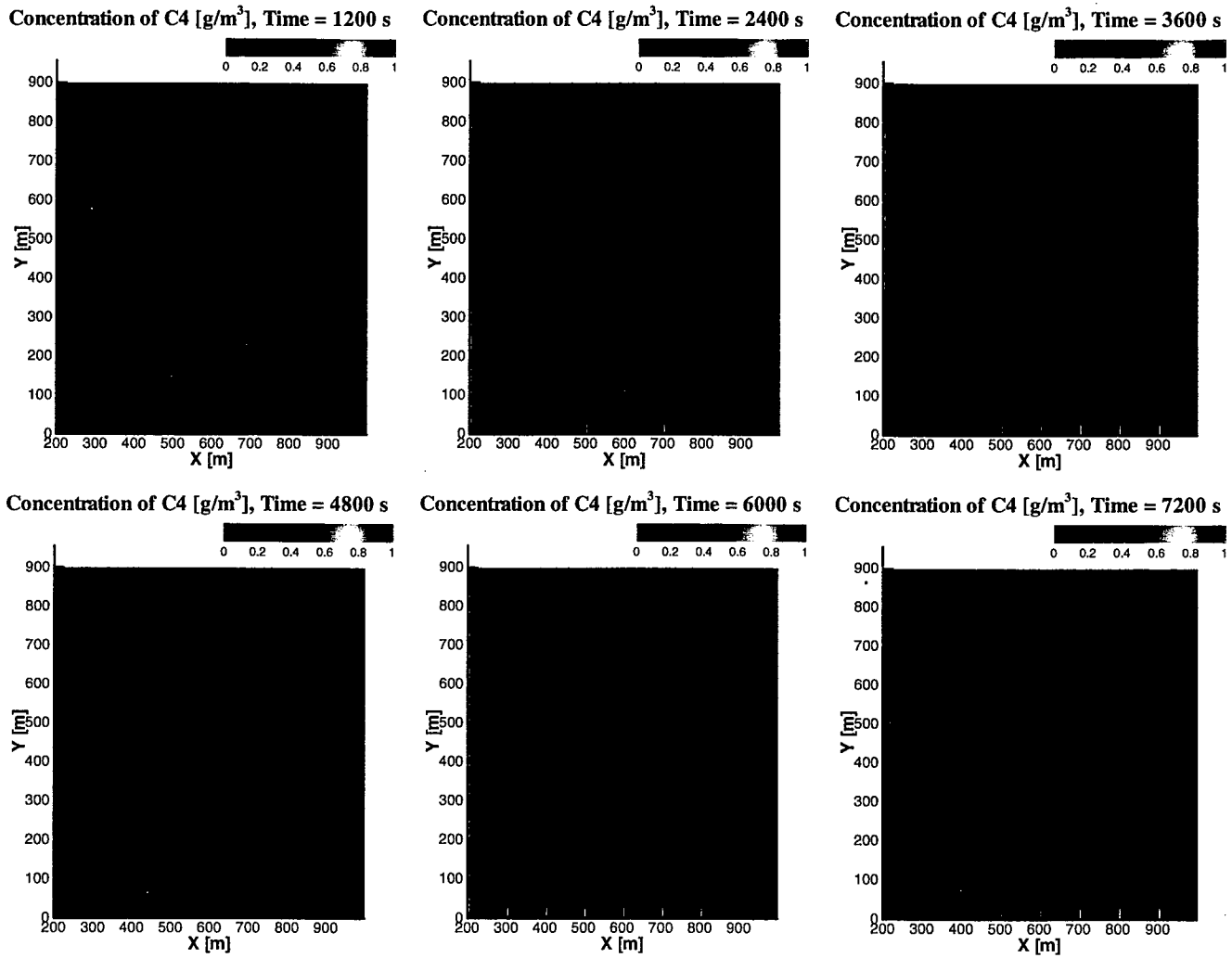


Figure 4.54. Concentration of the fourth dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport.

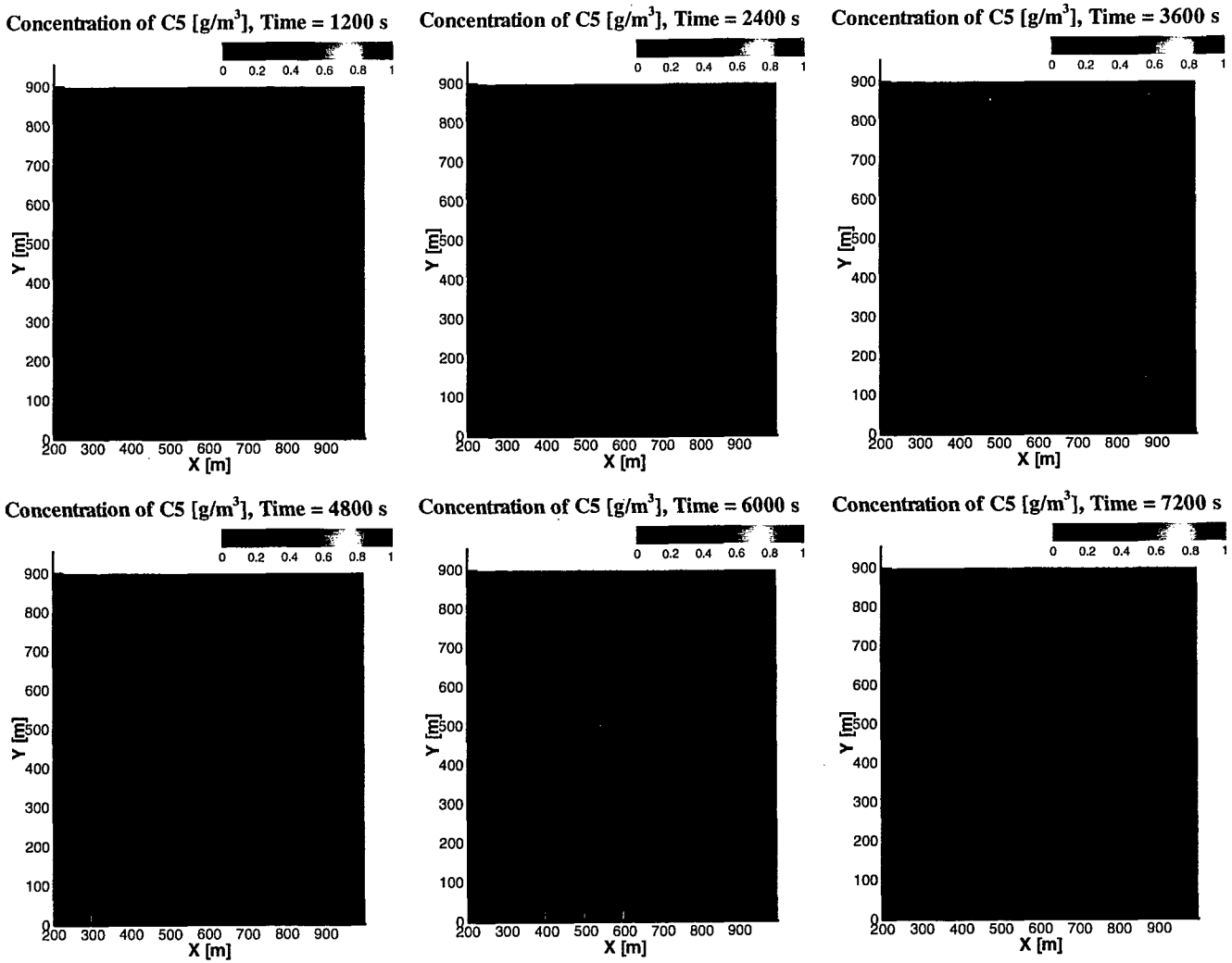


Figure 4.55. Concentration of the fifth dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport.

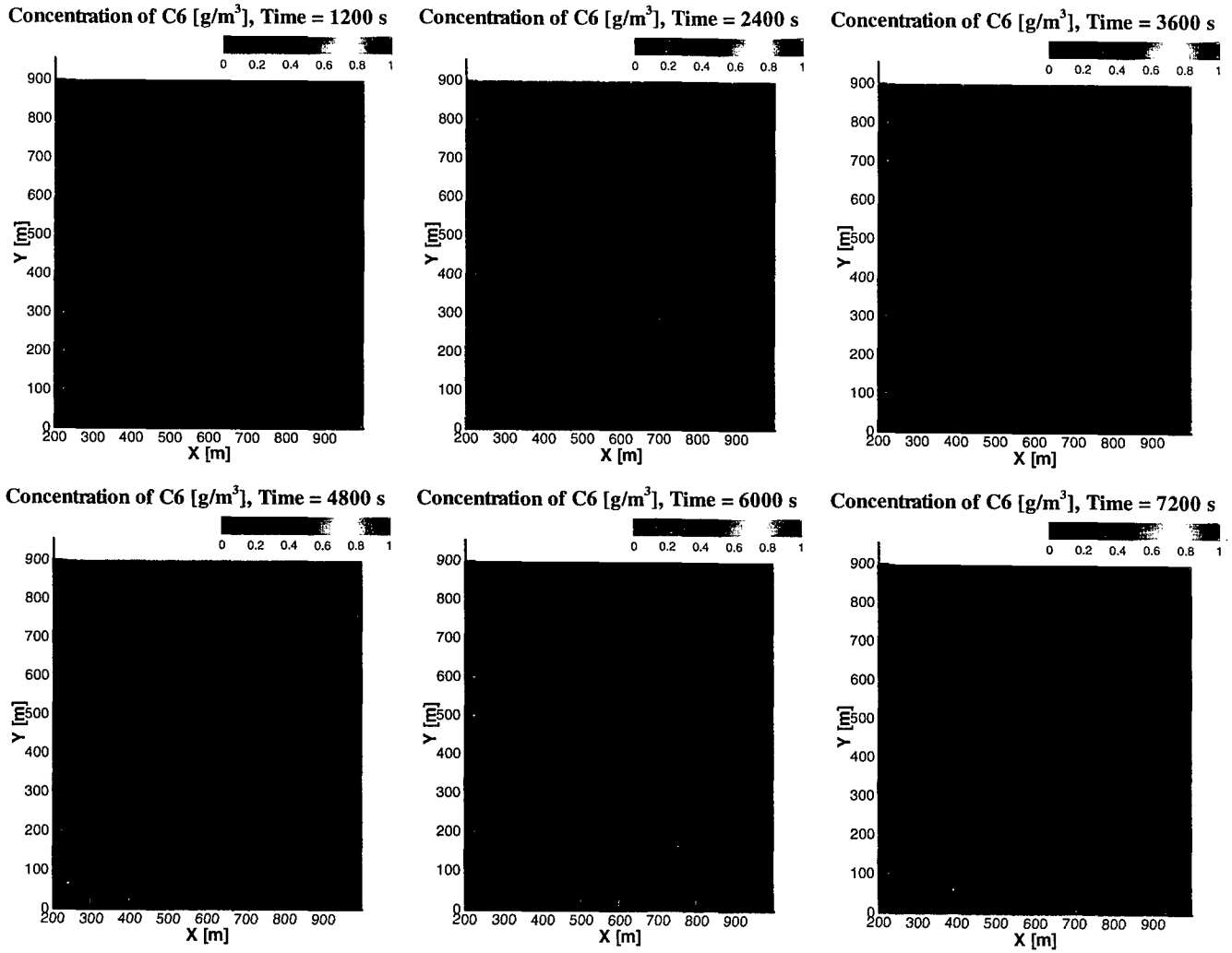


Figure 4.56. Concentration of the sixth dissolved chemical in 2-D overland at various times for the example of 1-D/2-D flow and transport.

5 SUMMARY AND CONTINUING WORK

A numerical model has been developed to simulate water flow and sediment and reactive chemical transport in watershed systems. The mathematical basis and numerical approaches of the model are given in Sections 2 and 3. Section 4 has demonstrated that the model was able to deal with various configurations of problems involving flow and sediment and chemical transport over watersheds with a wide range of ground surface slopes. Eight example problems were presented to illustrate the basic capability of the model.

Much experience has been gained throughout the research of this project. It was demonstrated that the method of characteristics can provide accurate numerical simulations in solving dynamic wave model when the slopes of ground surface are small. However, its application to solving problems with steep slopes has proved elusive. On the other hand, the Lagrangian approach was illustrated to be robust in solving diffusion and kinematic wave models. However, kinematic and diffusion wave models can yield accurate solutions only for cases of mild to steep slope problems. For cases of problems involving small slopes, the kinematic/diffusion wave models could not generate accurate results, even though the models can be solved easily. The kinematic wave model cannot even address the effects of backwater on flow dynamics over watersheds. In consideration of robustness (i.e., easy to solve with numerical methods) and accuracies, a hybrid model to adaptively choosing appropriate models (kinematic, diffusion, or dynamic wave models) for different regions of a watershed is much desirable.

Using the predictor-corrector approach to solving the transport equations, we have made the computation effective and robust. For each time, we need to solve the advection/dispersion transport only one time in the predictor step, and the chemical reaction system can be solved node by node in the corrector step. The reaction chemistry can be quite general. All reactions whose rates can be described by the collision theory are included in the model.

Continuing work is in progress to couple the watershed model with a three-dimensional subsurface flow and chemical transport model.

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APPENDIX A DATA INPUT GUIDE

This data input guide is composed of eight files: three for 2-D overland flow/transport, three for 1-D river/stream flow/transport, one for contaminant/sediment information and one for 1-D/2-D mapping. They are described as follows.

2-D Overland Geometry File (.2dm files for 2-D overland simulations)

T1-T3 Cards		Job title	
		Only one T1, T2, and T3 card can be used.	
GE Card		Element information	
Field	Variable	Value	Description
C 1-2	IC1	GE	Card group identifier.
C 3	IC3		Identification of element.
		3	A triangular element is being input.
		4	A quadrilateral element is being input.
1	M	+	id of global element.
2	IE1(M,1)	+	The index of node number 1 of the M element.
3	IE2(M,2)	+	The index of node number 2 of the M element.
4	IE2(M,3)	+	The index of node number 3 of the M element.
5	IE2(M,4)	+	The index of node number 4 of the M element. It is zero for a triangular element.
6	IE2(M,5)	+	id of the material type of the M element.
GN Card		Node information	
Field	Variable	Value	Description
C 1-2	IC1	GN	Card group identifier.
C 3	IC3		blank
1	N	+	id of global node..
2	X2(N,1)	+	The x-coordinate of the global node.
3	X2(N,2)	+	The y-coordinate of the global node.
4	X2(N,3)	+	The z-coordinate (bottom elevation) of the global node.
EN Card		End of data control	
Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

2-D Overland Flow File (.2bc files for 2-D overland simulations)

T1-T3 Cards	Job title
	Only one T1, T2, and T3 card can be used.

OP Card		Run option parameters	
Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	KMOD		Index of river/stream simulation.
		0	No river/stream simulation.
		1	Only flow is simulated.
		2	Both flow and transport are simulated.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMP		Index of using mass lumping.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTS		Index of using linear matrix solver for flow simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUAR		Index of using quadrature for numerical integration.
		1	Nodal quadrature for line element integration.
		2	Gaussian quadrature for line element integration.
4	IDIFF		Index of taking into account the eddy viscosity terms.
		1	Yes.
		0	No, the eddy viscosity terms are neglected.
5	IALLOW		Index of allowing the simulation to continue when there is no convergence reached for the non-linear iteration.
		1	Yes.
		0	No.
6	IMODEL		Index of simulating overland flow.
		3	Using MOC to solve the dynamic model only.
		2	Using the diffusion model only.
		1	Using the kinematic model only.
		0	Using the hybrid model .
		-10	Specifying water depth and flow velocity with the initial condition. The flow equation is not solved.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for simulations.
1	W		Time derivative weighting factor for flow simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OME		Relaxation parameter for solving nonlinear matrix equations.

		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.
3	OMI		Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGEN	0	GG will not be read.
		1	GG will be read.
2	GG	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	5	Method of characteristics.
1	ISK		Index of choosing the directions of characteristics.
		-1	Using the velocity direction as the direction of characteristics.
		0	Solve the diagonalization equations for the directions.
		1	Specify directions by users.
2	ANGLE1	+	User specified angle for the direction of the first characteristic. (COS(ANGLE1), SIN(ANGLE1)) is the direction.
3	ANGLE2	+	User specified direction for the second and third characteristics. (COS(ANGLE2), SIN(ANGLE2)) is the direction.

IP Card — Iteration Parameters

Field	Variable	Value	Description
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITER	+	Allowed number for the non-linear iteration in the flow simulation.
2	NPITER	+	Allowed number for the linearized iteration in the flow simulation.
3	TOLBH	+	Allowed relative error for water depth.
4	TOLBV	+	Allowed relative error for velocity components.
5	V_CUT	+	Cut-off of velocity. If the computed velocity is smaller than this value, it is set to zero.
6	FMSR	+	Multiplication factor to set the allowed mean square root errors, BHMSR for water depth and BVMSR for velocity, where BHMSR = TOLBH*FMSR; BVMSR = TOLBV*FMSR.

PT Card — Time marching parameters

Field	Variable	Value	Description

C 1-2	IC1	PT	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NXW	+	Subelement number in one direction that is used in the "in-element" particle tracking. The total subelement number included in one global element is NXW*NXW.
2	IDETQ		Index of particle tracking approach.
		1	Using the average-velocity approach.
		2	Using the constant-velocity approach.

TC Card — Iteration Parameters

Field	Variable	Value	Description
C 1-2	IC1	TC	Card group identifier.
C 3	IC3	1	Total simulation time.
1	TMAX	+	Maximum simulation time. [T]
2	DELT	+	Initial time step size. [T]

Field	Variable	Value	Description
C 1-2	IC1	TC	Card group identifier.
C 3	IC3	2	Computational time step.
1	IDTXY	+	Index of xy series for variable time step.

OC Card — Output control parameters

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	1	Print control parameters.
1	IBUG	0	Do not print the diagnostic output.
		1	Do print the diagnostic output.
2	JOPT	0	Print at specified intervals.
		1	Print at specified set of time values.
3	KPRT	+	Specify the interval if JOPT = 0.
	NPRINT	+	Specify total number of the specified times, if JOPT=1.

Note: NPRINT new lines after OC1 card are needed if JOPT = 1.

(the first new line)			
1	TPRT(1)	+	The 1-st specified time that the simulation results are to be printed.
(the second new line)			
1	TPRT(2)	+	The 2-nd specified time that the simulation results are to be printed.
	.		
(the NPRINT new line)			
1	TPRT(NPRINT)	+	The NPRINT-th specified time that the associated simulation results are to be printed.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier

C 3	IC3	2	Print options.
1	NSELT	+	Total options to be selected.
2	KPR0(i)		Print options.
		1	Print water depth.
		2	Print velocity.
		3	Print infiltration rate.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	3	Output control for post-process.
1	IFILE	0	Save as ascii format.
		1	Save as binary format.
2	KOPT	0	Save at specified interval.
		1	Save at specified set of times.
3	KDSK	+	Save every specified interval, if KOPT=0.
	NPOST	+	Save at specified set of times, if KOPT=1.

Note: NPOST new lines after OC3 card are needed if KOPT = 1.

(the first new line)			
1	TSV(1)	+	The 1-st specified time that the simulation results are to be saved.
(the second new line)			
1	TSV(2)	+	The 2-nd specified time that the simulation results are to be saved.
(the NPOST new line)			
1	TSV(NPOST)	+	The NPOST-th specified time that the simulation results are to be saved.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	4	Solution file output options.
1	KSELT	+	Total options to be selected.
2	KSAVE(i)		Save options.
		1	Save water depth.
		2	Save flux.
		3	Save infiltration rate.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	5	Print options for 1-D groundwater flow.
1	NCOLUM	+	Total vertical column to be printed.

Note: NCOLUM new lines after OC5 card are needed.

(the first new line)			
1	ICL(1)	+	The 1-st specified vertical column that the groundwater flow are to be printed.

(the second new line)

1	ICL(2)	+	The 2-nd specified vertical column that the groundwater flow are to be printed.

(the NPRINT new line)

1	ICL(NCOLUM)	+	The NCOLUM-th specified vertical column that the groundwater flow are to be printed.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	6	Print 1-D groundwater model options
1	NSELTG	+	Total options to be selected.
2	KPRG(i)		Print options.
		1	Print pressure head.
		2	Print water contents.
		3	Print velocity.

GC Card — Cross section parameters

Field	Variable	Value	Description
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	1	Generate cross section to calculate discharge.
1	NGCL	+	Total number of cross sections.

Field	Variable	Value	Description
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	2	Cross section information.
1	id	+	Index number of cross section.
2	NPL	+	Number of nodal points in the x-section.
(new line)		+	Node points.

Field	Variable	Value	Description
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	3	Save and print hydrograph.
1	LOPT	0	Save and print at specified interval.
		1	Save and print at specified set of times.
2	LDSK	0	Save and print at specified interval.
		+	Save and print every specified interval, if LOPT=0.
	LPOST	+	Save and print at specified set of times, if LOPT=1.

Note: LPOST new lines after GC3 card are needed if LOPT = 1.

(the first new line)

1	TSA(1)	+	The 1-st specified time that the hydrographs are to be saved.

(the second new line)

1	TSA(2)	+	The 2-nd specified time that the hydrographs are to be saved.

(the NPOST new line)

1	TSA(LPOST)	+	The LPOST-th specified time that the hydrographs are to be saved.
(new line)		+	After GC3 card, specify the times, if LOPT = 1. One data entry per line.

MP Card — Material property parameters

Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property.
1	i	+	id of material type.
2	PROP(1,i)	+	Manning's roughness associated with the material type.
3	PROP(2,i)	+	xx-eddy viscosity associated with the material type. [L^2/T]
4	PROP(3,i)	+	yy-eddy viscosity associated with the material type. [L^2/T]
5	PROP(4,i)	+	xy-eddy viscosity associated with the material type. [L^2/T]

Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	2	Density of water and acceleration of gravity.
1	ITUNIT		Index of time unit.
		1	The time unit for simulation is second.
		2	The time unit for simulation is minute.
		3	The time unit for simulation is hour.
2	ILUNIT		Index of length unit.
		1	The length unit for simulation is meter.
		2	The length unit for simulation is foot.
		3	The length unit for simulation is kilometer.
		4	The length unit for simulation is mile.
3	RHO	+	Density of water, (M/L^3).

SP Card — Soil property parameters

Field	Variable	Value	Description
C 1-2	IC1	SP	Card group identifier.
C 3	IC3	1	Index for computing the infiltration.
1	KSP		Index of infiltration rate.
		0	Input the infiltration rate.
		1	Computed by 1-D vertical groundwater model.

RF Card — Rainfall parameters

Field	Variable	Value	Description
C 1-2	IC1	RF	Card group identifier.
C 3	IC3	1	Rainfall data for the simulation.
1	i	+	id of global element.
2	IRTYP(i)	+	Index of the rainfall rate XY series for the element.

SS Card — Source/sink parameters

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	1	Source/sink data for the simulation.
1	i	+	id of global node.
2	ISR(i)	+	Index of the source/sink rate XY series for the node.

IN Card — Infiltration parameters

Field	Variable	Value	Description
C 1-2	IC1	IN	Card group identifier.
C 3	IC3	1	Input for Infiltration data.
1	i	+	id of global node.
2	ROUTND(i)	+	Input infiltration rate for the node. [L/T]

OB Card — Open boundary parameters

Field	Variable	Value	Description
C 1-2	IC1	OB	Card group identifier.
C3	IC3	1	Dirichlet boundary nodes for the simulation.
1	NPDB(j)	+	id of global node corresponding to the j-th Dirichlet boundary node.
2	IDTYP(j)	+	id of xy series to describe the time-dependent water surface elevation or water depth profile associated with the Dirichlet boundary node.
3	IDHB(j)		Index of the profile type for the j-th Dirichlet boundary node.
		0	Time-dependent water depth profile.
		1	Time-dependent water surface elevation profile.

Field	Variable	Value	Description
C 1-2	IC1	OB	Card group identifier.
C3	IC3	2	Flux-type boundary sides for the simulation.
1	NSCB(j,1)	+	id of global node corresponding to the 1-st node of the j-th flux-type boundary side.
2	NSCB(j,2)	+	id of global node corresponding to the 2-nd node of the j-th flux-type boundary side.
3	NSCB(j,3)		id of the type for the j-th flux-type boundary side.
		1	Upstream boundary with the incoming normal flux specified.
		2	Downstream boundary with the outgoing normal flux specified.
		3	This is either a river/stream-related or a river/stream junction-related boundary side with the water depth-dependent outgoing normal flux (when overland water and river/stream water are separated) or stage difference-dependent normal flux (when overland water and river or stream water are connected) specified.
4	ICTYP(j,1)	+	id of xy series to describe the time-dependent normal flux profile associated with the open boundary node when NSCB(j,3) = 1.
5	ICTYP(j,2)	+	id of xy series to describe the water depth-dependent normal flux profile associated with the open boundary node when NSCB(j,3) = 2,

			or 3 (for the case that river/stream and overland waters are separated).
6	ICTYP(j,3)	+	id of xy series to describe the water stage difference-dependent normal flux profile associated with the open boundary node when NSCB(j,3) = 3 (for the case that river/stream and overland waters are connected).

IC Card — Initial condition data parameters

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C3	IC3	H	Water depth or water surface elevation.
1	IHEAD	0	Constant water depth or water surface elevation.
		1	Variable water depth or water surface elevation.
2	IDHEAD	0	Initial water depth is input.
		1	Initial water surface elevation is input.
3	HCONST	+	Value of the constant water depth or water surface elevation for IHEAD = 0. [L]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C3	IC3	U	Velocity.
1	IV	0	Constant velocity.
		1	Variable velocity.
2	UCONST	+	Value of the constant velocity. [L/T]
3	VCONST	+	Value of the constant velocity. [L/T]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C3	IC3	S	Initial condition start type.
1	ISTART	0	Cold start, water depth/water surface elevation and velocity.
		1	Hot start, water surface elevation and velocity.

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C3	IC3	T	Initial condition start time.
1	HSTIME	+	Time corresponding for the hot start.

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C3	IC3	F	Initial condition start type.
1	ICFILE	0	Text format.
		1	Binary format.

XY Card — X-Y Series Parameters

Field	Variable	Value	Description
C 1-2	IC1	XY	Card group identifier.

C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

EN Card — End of data control

Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

2-D Overland Transport Files (.2tp files for 2-D overland simulations)

T1-T3 Cards — Job title

Only one T1, T2, and T3 card can be used.

OP Card — Run option parameters

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	IDCHEM		Index of chemical transport simulation.
		0	Chemical transport is not simulated.
		1	Chemical transport is simulated.
2	IDSED		Index of sediment transport simulation.
		0	Sediment transport is not simulated.
		1	Sediment transport is simulated.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMPT		Index of using mass lumping for transport simulations.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTST		Index of using linear matrix solver for transport simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUART		Index of using quadrature for numerical integration.
		1	Nodal quadrature for line element integration.

		2	Gaussian quadrature for line element integration.
4	IADAPT		Index of using adapted implicit-explicit scheme for the predictor step.
		0	No.
		1	Yes.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for transport simulations.
1	WT		Time derivative weighting factor for transport simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OMET		Relaxation parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.
3	OMIT		Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGENT	0	GGT will not be read.
		1	GGT will be read.
2	GGT	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

IP Card — Iteration Parameters

Field	Variable	Value	Description
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITERT	+	Allowed number for the non-linear iteration.
2	NPITER	+	Allowed number for the linearized iteration.
3	TOLBT	+	Allowed relative error for getting convergent transport solutions.

PT Card — Particle tracking parameters

Field	Variable	Value	Description
C 1-2	IC1	PT	Card group identifier.
C 3	IC3	1	Particle tracking controlling parameters.
1	NXWT	+	Subelement number in one direction that is used in the "in-element" particle tracking. The total subelement number included in one global element is NXWT*NXWT.
2	IDETQT		Index of particle tracking approach.

		1	Using the average-velocity approach.
		2	Using the constant-velocity approach.

MP Card — Material property parameters

Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property for transport.
1	i	+	id of material type.
2	PROPT(1,i)	+	Longitudinal dispersivity associated with the material type. [L]
3	PROPT(2,i)	+	Lateral dispersivity associated with the material type. [L]
4	PROPT(3,i)	+	Pure diffusion coefficient associated with the material type. [L^2/T]

SS card — Source/sink parameters

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	1	Source/sink profile for dissolved chemicals.
1	NP	+	id of global node.
2	j	+	id of dissolved chemical.
3	ITSR(NP,j)	+	Index of the source/sink XY series for dissolved chemical at the node.

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	2	Source/sink profile for suspended sediment.
1	NP	+	id of global node.
2	j	+	id of suspended sediment size.
3	NCHEM	+	Number of dissolved chemicals.
4	ITSR(m)	+	Index of the source/sink XY series for the suspended sediment size at the global node, where $m = NCHEM + j$.

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	3	Source/sink profile for particulate chemicals on suspended sediments.
1	NP	+	id of global node.
2	j	+	id of suspended sediment.
3	k	+	id of particulate chemical.
4	NCHEM	+	Number of dissolved chemicals.
5	NSSIZE	+	Number of sediment sizes.
6	ITSR(m)	+	Index of the source/sink XY series for the particulate chemical on the suspended sediment size at the global node, where $m = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1,NSSIZE]$, and $k \in [1, NCHEM]$.

DB Card — Dirichlet boundary parameters

Field	Variable	Value	Description
C 1-2	IC1	DB	Card group identifier.

C 3	IC3	1	Dirichlet boundary conditions for dissolved chemicals.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	i	+	id of dissolved Chemical.
4	IDTYPT(NP,i)	+	Index of the concentration XY series with the Dirichlet boundary node for the dissolved chemical.

Field	Variable	Value	Description
C 1-2	IC1	DB	Card group identifier.
C 3	IC3	2	Dirichlet boundary conditions for suspended sediments.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	k	+	id of suspended sediment size.
4	NCHEM	+	Number of dissolved chemicals.
5	IDTYPT(NP,i)	+	Index of the concentration XY series with the Dirichlet boundary node for the suspended sediment, *where i = NCHEM+k.*

Field	Variable	Value	Description
C 1-2	IC1	DB	Card group identifier.
C3	IC3	3	Dirichlet boundary conditions for particulate chemicals on suspended sediments.
1	NP	+	id of Dirichlet boundary node.
2	NPDBT(NP)	+	id of global node corresponding to the Dirichlet boundary node.
3	j	+	id of suspended sediment size.
4	k	+	id of particulate chemical.
5	NCHEM	+	Number of dissolved chemicals.
6	NSSIZE	+	Number of sediment sizes.
7	IDTYPT(NP,i)	+	Index of the concentration XY series for the particulate chemical on the suspended sediment, *where* $i = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1,NSSIZE]$, *and* $k \in [1, NCHEM]$.

FB Card — Flux-type boundary parameters

Field	Variable	Value	Description
C 1-2	IC1	FB	Card group identifier.
C 3	IC3	1	Flux-type boundary conditions for dissolved chemicals.
1	NS	+	id of flux-type boundary side.
2	NSCBT(NS,1)	+	id of global node corresponding to the 1-st node of the flux-type boundary side.
3	NSCBT(NS,2)	+	id of global node corresponding to the 2-nd node of the flux-type boundary side.
4	NSCBT(NS,3)		Index of boundary condition type for the flux-type boundary side.
		1	Variable boundary node with the concentration specified if the flow is incoming.
		2	Cauchy boundary node with Cauchy flux specified.

		3	Neumann boundary node Neumann flux specified.
		4	River/stream-related or a river/stream junction-related boundary node. The boundary condition is a Variable boundary condition. However, the concentrations along with the inward flow are not prescribed. Rather they are the concentrations at the river/stream node or river/stream junction for the time being.
5	i	+	id of dissolved Chemical.
6	ICTYPT(NS,i)	+	Index of the flux XY series at the flux-type boundary side for the dissolved chemical. It is a concentration profile when NSCBT(j,2) = 1, a Cauchy flux profile when NSCBT(j,2) = 2, and a Neumann flux profile when NSCBT(j,2) = 3.

Field	Variable	Value	Description
C 1-2	IC1	FB	Card group identifier.
C 3	IC3	2	Flux-type boundary conditions for suspended sediments.
1	NS	+	id of flux-type boundary side.
2	NSCBT(NS,1)	+	id of global node corresponding to the 1-st node of the flux-type boundary side.
3	NSCBT(NS,2)	+	id of global node corresponding to the 2-nd node of the flux-type boundary side.
4	NSCBT(NS,3)		Index of boundary condition type for the flux-type boundary side.
		1	Variable boundary node with the concentration specified if the flow is incoming.
		2	Cauchy boundary node with the Cauchy flux specified.
		3	Neumann boundary node with the Neumann flux specified.
		4	River/stream-related or a river/stream junction-related boundary node. The boundary condition is a Variable boundary condition. However, the concentrations along with the inward flow are not prescribed. Rather they are the concentrations at the river/stream node or river/stream junction for the time being.
5	k	+	id of suspended sediment size.
6	NCHEM	+	Number of dissolved chemicals.
7	ICTYPT(NS,i)	+	Index of the flux XY series at the flux-type boundary side for the suspended sediment, *where i = NCHEM+k.* It is a concentration profile when NSCBT(j,2) = 1, a Cauchy flux profile when NSCBT(j,2) = 2, and a Neumann flux profile when NSCBT(j,2) = 3.

Field	Variable	Value	Description
C 1-2	IC1	FB	Card group identifier.
C3	IC3	3	Flux-type boundary conditions for particulate chemicals on suspended sediments.
1	NS	+	id of flux-type boundary side.
2	NSCBT(NS,1)	+	id of global node corresponding to the 1-st node of the flux-type boundary side.

3	NSCBT(NS,2)+		id of global node corresponding to the 2-nd node of the flux-type boundary side.
4	NSCBT(NS,3)		Index of boundary condition type for the flux-type boundary side.
		1	Variable boundary node with the concentration specified if the flow is incoming.
		2	Cauchy boundary node with the Cauchy flux specified.
		3	Neumann boundary node with the Neumann flux specified.
		4	River/stream-related or a river/stream junction-related boundary node. The boundary condition is a Variable boundary condition. However, the concentrations along with the inward flow are not prescribed. Rather they are the concentrations at the river/stream node or river or stream junction for the time being.
5	j	+	id of suspended sediment size.
6	k	+	id of particulate chemical.
7	NCHEM	+	Number of dissolved chemicals.
8	NSSIZE	+	Number of sediment sizes.
9	ICTYPT(NS,i)+		Index of the flux XY series with the flux-type boundary side for the particulate chemical on the suspended sediment, *where i = NCHEM + NSSIZE + (j-1)*NCHEM + k, j ∈ [1,NSSIZE], and k ∈ [1, NCHEM].* It is a concentration profile when NSCBT(j,2) = 1, a Cauchy flux profile when NSCBT(j,2) = 2, and a Neumann flux profile when NSCBT(j,2) = 3.

RS card — Rainfall source parameters

Field	Variable	Value	Description
C 1-2	IC1	RS	Card group identifier.
C 3	IC3	1	Rainfall source profile for dissolved chemicals.
1	j	+	id of dissolved chemical.
2	IRC(j)	+	Index of the rainfall XY series for the dissolved chemical.

IC card — Initial condition parameters

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	1	Initial condition parameters.
1	IDCONC		id of initial concentrations.
		0	constant initial concentrations.
		1	variable initial concentrations.

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	2	Initially constant conditions for dissolved chemicals.
1	j	+	id of the dissolved chemical being input.
2	CCONST(j)	+	Specified initial concentration for the dissolved chemical. [M/L^3]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	3	Initially constant conditions for particulate chemicals on suspended sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the suspended sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	CCONST(k)	+	Specified initial concentration for the particulate chemical on suspended sediment being input, where k = i*NCHEM + j. [M/M]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	4	Initially constant conditions for particulate chemicals on bed sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the bed sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	NSSIZE	+	Number of sediment sizes.
5	CCONST(k)	+	Specified initial concentration for the particulate chemical on the bed sediment being input, where k = (i+NSSIZE)* NCHEM + j. [M/M]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	5	Initially constant conditions for suspended sediments.
1	i	+	id of the suspended sediment size being input.
2	SCONST(i)	+	Specified initial concentration for the suspended sediment of the i-th size. [M/L^3]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	6	Initially constant conditions for bed sediments.
1	i	+	id of the bed sediment size being input.
2	NSSIZE	+	Number of sediment sizes.
3	SCONST(k)	+	Specified initial concentration for the bed sediment of the i-th size, where k = NSSIZE + i. [M/L^3]

XY Card — X-Y Series Parameters

Field	Variable	Value	Description
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.
5	REPEAT	0	Dummy values.

6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

EN Card		End of data control	
Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

1-D River/stream Geometry File (.2dm files for 1-D river/stream simulations)

T1-T3 Cards	Job title
	Only one T1, T2, and T3 card can be used.

GE Card		Element information	
Field	Variable	Value	Description
C 1-2	IC1	GE	Card group identifier.
C 3	IC3	2	Identification of element.
1	M	+	id of global element.
2	IE1(M,1)	+	The index of node number 1 of the M element
3	IE1(M,2)	+	The index of node number 2 of the M element
4	IE1(M,3)	+	id of the material type of the global element.

GN Card		Node information	
Field	Variable	Value	Description
C 1-2	IC1	GN	Card group identifier.
C 3	IC3		blank.
1	N	+	id of Global node.
2	X1(N,1)	+	The x-coordinate of the global node.
3	X1(N,2)	+	The z-coordinate (bottom elevation) of the global node.

EN Card		End of data control	
Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

1-D River/stream Flow File (.2bc files for 1-D river/stream simulations)

T1-T3 Cards	Job title
	Only one T1, T2, and T3 card can be used.

OP Card		Run option parameters	
Field	Variable	Value	Description

C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	KMOD		Index of river/stream simulation.
		0	No river/stream simulation.
		1	Only flow is simulated.
		2	Both flow and transport are simulated.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMP		Index of using mass lumping.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTS		Index of using linear matrix solver for flow simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial),
		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUAR		Index of using quadrature for numerical integration.
		1	Nodal quadrature for line element integration.
		2	Gaussian quadrature for line element integration.
4	IDIFF		Index of taking into account the eddy viscosity terms.
		1	Yes.
		0	No, the eddy viscosity terms are neglected.
5	IALLOW		Index of allowing the simulation to continue when there is no convergence reached for the non-linear iteration.
		1	Yes.
		0	No.
6	IMODEL		Index of simulating overland flow.
		3	Using MOC to solve the dynamic model only.
		2	Using the diffusion model only.
		1	Using the kinematic model only.
		0	Using the hybrid model .
		-10	Specifying water depth and velocity as the initial conditions. The flow equation is not solved.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for simulations.
1	W		Time derivative weighting factor for flow simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OME		Relaxation parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.

		1.0-2.0	Over relaxation.
3	OMI		Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGEN	0	GGT will not be read.
		1	GGT will be read.
2	GG	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

IP Card — Iteration Parameters

Field	Variable	Value	Description
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITER	+	Allowed number for the non-linear iteration in the flow simulation.
2	NPITER	+	Allowed number for the linearized iteration in the flow simulation.
3	TOLBH	+	Allowed relative error for water depth.
4	TOLBV	+	Allowed relative error for velocity components.
5	V_CUT	+	Cut-off of velocity. If the computed velocity is smaller than this value, it is set to zero.
6	FMSR	+	Multiplication factor to set the allowed mean square root errors, BHMSR for water depth and BVMSR for velocity, where BHMSR = TOLBH*FMSR; BVMSR = TOLBV*FMSR.

PT Card — Particle tracking parameters

Field	Variable	Value	Description
C 1-2	IC1	PT	Card group identifier.
C 3	IC3	1	Particle tracking controlling parameters.
1	NXW	+	Subelement number used in the x-direction in the "in-element" particle tracking.
2	IDETQ		Index of particle tracking approach.
		1	Using the average-velocity approach.
		2	Using the constant-velocity approach.

TC Card — Iteration Parameters

Field	Variable	Value	Description
C 1-2	IC1	TC	Card group identifier.
C 3	IC3	1	Total simulation time.
1	TMAX	+	Maximum simulation time. [T]
2	DELT	+	Initial time step size. [T]

Field	Variable	Value	Description
C 1-2	IC1	TC	Card group identifier.
C 3	IC3	2	Computational time step.
1	IDTXY	+	Index of xy series for variable time step.

OC Card		Output control parameters	
Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	1	Print control parameters.
1	IBUG	0	Do not print the diagnostic output.
		1	Do print the diagnostic output.
2	JOPT	0	Print at specified interval.
		1	Print at specified set of time values.
3	KPRT	+	Specify the interval if JOPT = 0.
	NPRINT	+	Specify total number of the specified times, if JOPT=1.

Note: NPRINT new lines after OC1 card are needed if JOPT = 1.

(the first new line)			
1	TPRT(1)	+	The 1-st specified time that the simulation results are to be printed.
(the second new line)			
1	TPRT(2)	+	The 2-nd specified time that the simulation results are to be printed.
(the NPRINT new line)			
1	TPRT(NPRINT)	+	The NPRINT-th specified time that the simulation results are to be printed.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier
C 3	IC3	2	Print options.
1	NSELT	+	Total options to be selected.
2	KPR0(i)		Print options.
		1	Print water depth.
		2	Print velocity.
		3	Print infiltration rate.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	3	Output control for post-process.
1	IFILE	0	Save as ascii format.
		1	Save as binary format.
2	KOPT	0	Save at specified interval.
		1	Save at specified set of times.
3	KDSK	+	Save every specified interval, if KOPT=0.
	NPOST	+	Save at specified set of times, if KOPT=1.

Note: NPOST new lines after OC3 card are needed if KOPT = 1.

(the first new line)			
1	TSV(1)	+	The 1-st specified time that the simulation results are to be saved.
(the second new line)			
1	TSV(2)	+	The 2-nd specified time that the simulation results are to be saved.
(the NPOST new line)			
1	TSV(NPOST)	+	The NPOST-th specified time that the simulation results are to be saved.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	4	Solution file output options.
1	KSELT	+	Total options to be selected.
2	KSAVE(i)		Save options.
		1	Save water depth.
		2	Save flux.
		3	Save infiltration rate.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	5	Print options for 1-D groundwater flow.
1	NCOLUM	+	Total vertical column to be printed.

Note: NCOLUM new lines after OC5 card are needed.

(the first new line)			
1	ICL(1)	+	The 1-st specified vertical column that the groundwater flow are to be printed.
(the second new line)			
1	ICL(2)	+	The 2-nd specified vertical column that the groundwater flow are to be printed.
(the NPRINT new line)			
1	ICL(NCOLUM)	+	The NCOLUM-th specified vertical column that the groundwater flow are to be printed.

Field	Variable	Value	Description
C 1-2	IC1	OC	Card group identifier.
C 3	IC3	6	Print 1-D groundwater model options.
1	NSELTG	+	Total options to be selected.
2	KPRG(i)		Print options.
		1	Print pressure head.
		2	Print water contents.
		3	Print velocity.

GC Card Cross section parameters

Field	Variable	Value	Description
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	1	Generate cross section to calculate discharge.
1	NGCL	+	Total number of cross sections.

Field	Variable	Value	Description
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	2	Cross section information.
1	id	+	Index number of cross section.
2	NPL	+	Number of nodal points in the x-section.
(new line)		+	Node points.

Field	Variable	Value	Description
C 1-2	IC1	GC	Card group identifier.
C 3	IC3	3	Save and print hydrograph.
1	LOPT	0	Save and print at specified interval.
		1	Save and print at specified set of times.
2	LDSK	0	Save and print at specified interval.
		+	Save and print every specified interval, if LOPT=0.
	LPOST	+	Save and print at specified set of times, if LOPT=1.

Note: LPOST new lines after GC3 card are needed if LOPT = 1.

(the first new line)			
1	TSA(1)	+	The 1-st specified time that the hydrographs are to be saved.
(the second new line)			
1	TSA(2)	+	The 2-nd specified time that the hydrographs are to be saved.
(the NPOST new line)			
1	TSA(LPOST)	+	The LPOST-th specified time that the hydrographs are to be saved.
(new line)		+	After GC3 card, specify the times, if LOPT = 1. One data entry per line.

MP Card — Material property parameters

Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property.
1	i	+	id of material type.
2	PROP(1,i)	+	Manning's roughness associated with the material type.
3	PROP(2,i)	+	x-eddy viscosity associated with the material type. [L^2/T]

Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	2	Density of water and acceleration of gravity.
1	ITUNIT		Index of time unit.
		1	The time unit for simulation is second.

		2	The time unit for simulation is minute.
		3	The time unit for simulation is hour.
2	ILUNIT		Index of length unit.
		1	The length unit for simulation is meter.
		2	The length unit for simulation is foot.
		3	The length unit for simulation is kilometer.
		4	The length unit for simulation is mile.
3	RHO	+	Density of water. [M/L^3]

SP Card — Soil property parameters

Field	Variable	Value	Description
C 1-2	IC1	SP	Card group identifier.
C 3	IC3	1	Index for computing the infiltration.
1	KSP		Index of infiltration rate.
		0	Input the infiltration rate.
		1	Computed by 1-D vertical groundwater model.

RF Card — Rainfall parameters

Field	Variable	Value	Description
C 1-2	IC1	RF	Card group identifier.
C 3	IC3	1	Rainfall data for the simulation.
1	i	+	id of global element.
2	IRTYP(i)	+	Index of the rainfall XY series for the element.

SS Card — Source/sink parameters

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	1	Source/sink data for the simulation.
1	i	+	id of global node.
2	ISR(i)	+	Index of the source/sink XY series for the node.

IN Card — Infiltration parameters

Field	Variable	Value	Description
C 1-2	IC1	IN	Card group identifier.
C 3	IC3	1	Input for Infiltration data.
1	i	+	id of global node.
2	ROUTND(i)	+	Input infiltration rate for the node. [L/T]

OB Card — Open boundary parameters

Field	Variable	Value	Description
C 1-2	IC1	OB	Card group identifier.
C 3	IC3	1	Open boundary for the simulation.
1	NPDB(j,1)	+	id of global node corresponding to the j-th open boundary node.
2	NPDB(j.2)		id of the type for the open boundary node.

		1	Boundary node with the water surface elevation specified.
		2	Upstream boundary node with the incoming normal flux specified.
		3	Downstream boundary node with the outgoing normal flux specified.
3	IDTYP(j,1)	+	id of xy series to describe the water surface elevation or water depth profile associated with the open boundary node when NPDB(j,2) = 1.
4	IDTYP(j,2)	+	id of xy series to describe the normal flux profile associated with the open boundary node when NPDB(j,2) = 2.
5	IDTYP(j,3)	+	id of xy series to describe the water depth-dependent normal flux profile associated with the open boundary node when NPDB(j,2) = 3.
6	IDHB(j)		Index of the profile type for IDTYP(j,2) when NPDB(j,2) = 2.
		0	Time-dependent water depth profile.
		1	Time-dependent water surface elevation profile.

CS Card — River/stream cross-sectional parameters

Field	Variable	Value	Description
C 1-2	IC1	CS	Card group identifier.
C 3	IC3	1	Profile types for river/stream cross-sectional geometry.
1	j	+	id of river/stream node.
2	ICHN(j,1)	+	id of xy series to describe the water depth-dependent cross-sectional area profile for the river/stream node.
3	ICHN(j,2)	+	id of xy series to describe the water depth-dependent wetted perimeter profile for the river/stream node.
4	ICHN(j,3)	+	id of xy series to describe the water depth-dependent top river/stream width profile for the river/stream node.

Note: The top river/stream width value at zero water depth must be GREATER than zero when describing the profile associated with it.

Field	Variable	Value	Description
C 1-2	IC1	CS	Card group identifier.
C 3	IC3	2	Entire river/stream width .
1	j	+	id of river/stream node.
2	CHNW(j)	+	The entire river/stream width through which rainfall can contribute to river/stream at the river/stream node. [L]

RH Card — River/stream reach parameters

Field	Variable	Value	Description
C 1-2	IC1	RH	Card group identifier.
C 3	IC3	1	River/stream nodes included in each river/stream reach.
1	j	+	id of river/stream reach.
2	nn	+	Number of nodes included in the river/stream reach.

Note: A river/stream reach must include at least four river/stream nodes. One new line after RH1 card is needed.

(new line, including nn data)

NPINRH(1..nn,j)	+	Node numbers of river/stream nodes that are included in the river/stream reach. These nodes must be given in order from the upstream to the downstream.

JT Card — River/stream junctions

Field	Variable	Value	Description
C 1-2	IC1	JT	Card group identifier.
C3	IC3	1	parameters of junction geometry.
1	j	+	id of river/stream junction.
2	NPJT(j)	+	id of overland global node that is associated with the j-th junction.
3	IVJT(j)	+	id of xy series to describe the volume-water depth relation at the river/stream junction.
4	IDJCNT(j)	1	This junction is to simulate a big lake and the water stage at junction's outlets are considered to be the same as the junction's.
		0	Otherwise.
5	AJT(j)	+	Horizontal area of the junction, through which both rainfall and infiltration can contribute to the change of water depth of the junction. [L^2]
6	Z0JT(j)	+	Bottom elevation of the junction. [L]

Field	Variable	Value	Description
C 1-2	IC1	JT	Card group identifier.
C3	IC3	2	river/stream reaches and nodes associated with river/stream junctions.
1	j		id of river/stream junction.
2	NJTRH(j)	+	Number of river/stream reaches that connect to one another through the river/stream junction.

Note: If this river/stream junction is simulating a pond without outlet, NJTRH(j) = 0.

(new line) IDJT(1,1..nn,j)		id of river/stream global nodes which coincide with the junction and are the end nodes of the reaches connected to the junction. (nn = NJTRH(j))
(new line) DJT(2,1..nn,j)		id of river/stream global nodes which are the nodes next to the nodes specified in IDJT(1,1..nn,j). (nn = NJTRH(j))

Note: IDJT(1,i,j) must match IDJT(2,i,j) for the i-th reach connected to the j-th junction.

Field	Variable	Value	Description
C 1-2	IC1	JT	Card group identifier.
C3	IC3	3	junction-related overland boundary sides.
1	j	+	id of river/stream junction.

Note: A river/stream dead end is treated as a river/stream junction.

2	NJT12(j)	+	Number of junction-related overland boundary segments.

Note: nn new lines after JT3 card are needed, where nn = NJT12(j).

(the first new line)			
1	NSJT12(1,1)	+	The 2D global node that corresponds to the 1-st node of the 1-st

			surrounding overland boundary segment of the river/stream junction.
2	NSJT12(2,1)	+	The 2D global node that corresponds to the 2-nd node of the 1-st surrounding overland boundary segment of the river/stream junction.
(the nn-th new line)			
1	NSJT12(1,nn)	+	The 2D global node that corresponds to the 1-st node of the nn-th surrounding overland boundary segment of the river/stream junction.
2	NSJT12(2,nn)	+	The 2D global node that corresponds to the 2-nd node of the nn-th surrounding overland boundary segment of the river/stream junction.

IC Card — Initial condition data parameters

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C3	IC3	H	Water depth or water surface elevation.
1	IHEAD	0	Constant water depth or water surface elevation.
		1	Variable water depth or water surface elevation.
2	IDHEAD	0	Initial water depth is input.
		1	Initial water surface elevation is input.
3	HCONST	+	Value of the constant water depth or water surface elevation for IHEAD = 0. [L]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	U	Velocity.
1	IV	0	Constant velocity.
		1	Variable velocity.
2	UCONST	+	Value of the constant velocity. [L/T]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	S	Initial condition start type.
1	ISTART	0	Cold start, water depth/water surface elevation and velocity.
		1	Hot start, water surface elevation and velocity.

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	T	Initial condition start time.
1	HSTIME	+	Time corresponding for the hot start.

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	F	Initial condition start type.
1	ICFILE	0	Text format.
		1	Binary format.

XY Card		X-Y Series Parameters	
Field	Variable	Value	Description
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line) X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

EN Card		End of data control	
Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

1-D River/stream Transport File (.2tp files for 2-D overland simulations)

T1-T3 Cards		Job title	
		Only one T1, T2, and T3 card can be used.	

OP Card		Run option parameters	
Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	1	Simulation selection.
1	IDCHEM		Index of chemical transport simulation.
		0	Chemical transport is not simulated.
		1	Chemical transport is simulated.
2	IDSED		Index of sediment transport simulation.
		0	Sediment transport is not simulated.
		1	Sediment transport is simulated.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	2	Solver specification.
1	ILUMPT		Index of using mass lumping for transport simulations.
		0	No mass lumping.
		1	Mass lumping.
2	IPNTST		Index of using linear matrix solver for transport simulations.
		1	The pointwise iterative matrix solver.
		2	Preconditioned Conjugate Gradient Method (polynomial),

		3	Preconditioned Conjugate Gradient Method (Incomplete Cholesky).
3	IQUART		Index of using quadrature for numerical integration.
		1	Nodal quadrature for line element integration.
		2	Gaussian quadrature for line element integration.
4	IADAPT		Index of using adapted implicit-explicit scheme for the predictor step.
		0	No.
		1	Yes.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	3	Weighting factor for transport simulations.
1	WT		Time derivative weighting factor for transport simulation.
		0.5	Crank-Nicolson central.
		1.0	Backward difference.
2	OMET		Relaxation parameter for solving nonlinear matrix equations.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.
3	OMIT		Relaxation parameter for solving linearized matrix equation.
		0.0-1.0	Under relaxation.
		1.0	Exact relaxation.
		1.0-2.0	Over relaxation.

Field	Variable	Value	Description
C 1-2	IC1	OP	Card group identifier.
C 3	IC3	4	Preconditioned Conjugate Gradient method.
1	IEIGENT	0	GGT will not be read.
		1	GGT will be read.
2	GGT	+	Upper bound of the maximum eigenvalue of the coefficient matrix used in the Preconditioned Conjugate Gradient method.

IP Card — Iteration Parameters

Field	Variable	Value	Description
C 1-2	IC1	IP	Card group identifier.
C 3	IC3	1	Total simulation time.
1	NNITERT	+	Allowed number for the non-linear iteration.
2	NPITER	+	Allowed number for the linearized iteration.
3	TOLBC	+	Allowed relative error for getting convergent transport solutions for both dissolved and particulate chemicals.
4	TOLBS	+	Allowed relative error for getting convergent transport solutions for sediments.

PT Card — Particle tracking parameters

Field	Variable	Value	Description

C 1-2	IC1	PT	Card group identifier.
C 3	IC3	1	Particle tracking controlling parameters.
1	NXWT	+	Subelement number used in the x-direction in the "in-element" particle tracking.
2	IDETQT		Index of particle tracking approach.
		1	Using the average-velocity approach.
		2	Using the constant-velocity approach.

MP Card — Material property parameters

Field	Variable	Value	Description
C 1-2	IC1	MP	Card group identifier.
C 3	IC3	1	Material property for transport.
1	i	+	id of material type.
2	PROPT(1,i)	+	Longitudinal dispersivity associated with the material type. [L]
3	PROPT(2,i)	+	Pure diffusion coefficient associated with the material type. [L^2/T]

SS card — Source/sink parameters

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	1	Source/sink profile for dissolved chemicals.
1	NP	+	id of global node.
2	j	+	id of dissolved chemical.
3	ITSR(NP,j)	+	Index of the source/sink XY series for the dissolved chemical at the global node.

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	2	Source/sink profile for suspended sediment.
1	NP	+	id of global node.
2	j	+	id of suspended sediment size.
3	NCHEM	+	Number of dissolved chemicals.
4	ITSR(NP,m)	+	Index of the source/sink XY series for the suspended sediment size at the global node, where $m = NCHEM + j$.

Field	Variable	Value	Description
C 1-2	IC1	SS	Card group identifier.
C 3	IC3	3	Source/sink profile for particulate chemicals on suspended sediments.
1	NP	+	id of global node.
2	j	+	id of suspended sediment.
3	k	+	id of particulate chemical.
4	NCHEM	+	Number of dissolved chemicals.
5	NSSIZE	+	Number of sediment sizes.
6	ITSR(NP,m)	+	Index of the source/sink XY series for the particulate chemical on the suspended sediment size at the global node, where $m = NCHEM +$

*NSSIZE + (j-1)*NCHEM + k, j ∈ [1,NSSIZE],* and *k ∈ [1, NCHEM].*

UB Card		User-specified boundary parameters	
Field	Variable	Value	Description
C 1-2	IC1	UB	Card group identifier.
C 3	IC3	1	User-specified boundary conditions for dissolved chemicals.
1	NP	+	id of user-specified boundary node.
2	NPDBT(NP,1)	+	id of global node corresponding to the user-specified boundary node.
3	NPDBT(NP,2)		Index of boundary condition type for the user-specified boundary node.
		1	Dirichlet boundary node with the concentration specified.
		2	Variable boundary node with th concentration specified if the flow is incoming.
		3	Cauchy boundary node with the Cauchy flux specified.
		4	Neumann boundary node with Neumann flux specified.
4	i	+	id of dissolved Chemical.
5	IDTYPT(NP,i)	+	Index of the XY series associated with the user-specified boundary node for the dissolved chemical. It is a concentration profile when NPDB(j,2) = 1, a concentration profile when NPDB(j,2) = 2, a Cauchy flux profile when NPDB(j,2) = 3, and a Neumann flux profile when NPDB(j,2) = 4.

Field	Variable	Value	Description
C 1-2	IC1	UB	Card group identifier.
C 3	IC3	2	User-specified boundary conditions for suspended sediments.
1	NP	+	id of user-specified boundary node.
2	NPDBT(NP,1)	+	id of global node corresponding to the user-specified boundary node.
3	NPDBT(NP.2)		Index of boundary condition type for the user-specified boundary node.
		1	Dirichlet boundary node with the concentration specified.
		2	Variable boundary node with the concentration specified if the flow is incoming.
		3	Cauchy boundary node with the Cauchy flux specified.
		4	Neumann boundary node with the Neumann flux specified.
4	k	+	id of suspended sediment size.
5	NCHEM	+	Number of dissolved chemicals.
6	IDTYPT(NP,i	+	Index of the XY series associated with the user-specified boundary node for the suspended sediment, *where i = NCHEM+k.* It is a concentration profile when NPDBT(j,2) = 1, a concentration profile when NPDBT(j,2) = 2, a Cauchy flux profile when NPDBT(j,2) = 3, and a Neumann flux profile when NPDBT(j,2) = 4.

Field	Variable	Value	Description
C 1-2	IC1	UB	Card group identifier.
C3	IC3	3	User-specified boundary conditions for particulate chemical.on suspended sediments.

1	NP	+	id of user-specified boundary node.
2	NPDBT(NP,1)	+	id of global node corresponding to the user-specified boundary node.
3	NPDBT(NP,2)		Index of boundary condition type for the user-specified boundary node.
		1	Dirichlet boundary node with the concentration specified.
		2	Variable boundary node with the concentration specified if the flow is incoming.
		3	Cauchy boundary node with the Cauchy flux specified.
		4	Neumann boundary node with the Neumann flux specified.
4	j	+	id of suspended sediment size.
5	k	+	id of particulate chemical.
6	NCHEM	+	Number of dissolved chemicals.
7	NSSIZE	+	Number of sediment sizes.
8	IDTYPT(NP,i)	+	Index of the XY series associated with the user-specified boundary node for the particulate chemical on the suspended sediment, *where* $i = NCHEM + NSSIZE + (j-1)*NCHEM + k$, $j \in [1,NSSIZE]$, *and* $k \in [1, NCHEM]$. It is a concentration profile when NPDBT(j,2) = 1, a concentration profile when NPDBT(j,2) = 2, a Cauchy flux profile when NPDBT(j,2) = 3, and a Neumann flux profile when NPDBT(j,2) = 4.

RS card — Rainfall source parameters

Field	Variable	Value	Description
C 1-2	IC1	RS	Card group identifier.
C 3	IC3	1	Rainfall source profile for dissolved chemicals.
1	j	+	id of dissolved chemical.
2	IRC(j)	+	Index of the rainfall XY series for the dissolved chemical.

IC card — Initial condition parameters

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	1	Initial condition parameters.
1	IDCONC		id of initial concentrations.
		0	constant initial concentrations.
		1	variable initial concentrations.

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	2	Initially constant conditions for dissolved chemicals
1	j	+	id of the dissolved chemical being input.
2	CCONST(j)	+	Specified initial concentration for the dissolved chemical. [M/L^3]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	3	Initially constant conditions for particulate chemicals on suspended

			sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the suspended sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	CCONST(k)	+	Specified initial concentration for the particulate chemical on suspended sediment being input, where k = i*NCHEM + j. [M/M]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	4	Initially constant conditions for particulate chemicals on bed sediments
1	j	+	id of the particulate chemical being input.
2	i	+	id of the bed sediment size where the particulate chemical is.
3	NCHEM	+	Number of dissolved chemicals.
4	NSSIZE	+	Number of sediment sizes.
5	CCONST(k)	+	Specified initial concentration for the particulate chemical on the bed sediment being input, where k = (i+NSSIZE)* NCHEM + j. [M/M]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	5	Initially constant conditions for suspended sediments.
1	i	+	id of the suspended sediment size being input.
2	SCONST(i)	+	Specified initial concentration for the suspended sediment ofthe i-th size. [M/L^3]

Field	Variable	Value	Description
C 1-2	IC1	IC	Card group identifier.
C 3	IC3	6	Initially constant conditions for bed sediments.
1	i	+	id of the bed sediment size being input.
2	NSSIZE	+	Number of sediment sizes.
3	SCONST(k)	+	Specified initial concentration for the bed sediment of the i-th size, where k = NSSIZE + i. [M/L^3]

XY Card — X-Y Series Parameters

Field	Variable	Value	Description
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line

up to NPOINT(i).

EN Card		End of data control	
Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

1-D/2-D Contaminant/sediment File (.2ch files for transport simulations)

T1-T3 Cards		Job title	
		Only one T1, T2, and T3 card can be used.	

RX card		Chemical reaction parameters	
Field	Variable	Value	Description
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	1	Numbers of reactions and chemicals
1	NRXN	+	Number of reactions.
2	NCHEM	+	Number of dissolved chemicals.

Field	Variable	Value	Description
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	2	Chemical names
1	NCHEM	+	Number of dissolved Chemical.

Note: NCHEM new lines are needed.

(the first new line)		
CHEMN(1)	+	Name of the 1-st dissolved chemical.
(the second new line)		
CHEMN(2)	+	Name of the 2-nd dissolved chemical.
(the NCHEM-th new line)		
CHEMN(NCHEM)	+	Name of the NCHEM-th dissolved chemical.

Field	Variable	Value	Description
C 1-2	IC1	RX	Card group identifier.
C 3	IC3	3	Reaction rate constants and stoichiometry
1	j	+	id of chemical reaction.
2	NCHEM	+	Number of dissolved chemicals.
3	FKRX(j)	+	Forward reaction rate constant of the reaction. [reaction dependent]
4	BKRX(j)	+	Backward reaction rate constant of the reaction. [reaction dependent]

Note: Two new lines are needed.

(the first new line)			
1	NURTS(j,1)	+	Stoichiometric coefficient of the 1-st dissolved chemical (on the reactant side) in the reaction.
2	NURTS(j,2)	+	Stoichiometric coefficient of the 2-nd dissolved chemical (on the

reactant side) in the reaction.

up to NURTS(j,NCHEM)
(the second new line)

1	NUPDS(j,1)	+	Stoichiometric coefficient of the 1-st dissolved chemical (on the product side) in the reaction.
2	NUPDS(j,2)	+	Stoichiometric coefficient of the 2-nd dissolved chemical (on the product side) in the reaction.

up to NUPDS(j,NCHEM)

ST card — Sediment parameters

Field	Variable	Value	Description
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	1	Number of sediment sizes
1	NSSIZE	+	Number of sediment sizes.

Field	Variable	Value	Description
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	2	Parameter associated with each sediment size.
1	j	+	id of Sediment size.
2	SPARA(j,1)		The type of the sediment size.
		1	Cohesive sediment, e.g., clay and silt.
		2	Non-cohesive sediment, e.g., sand.
3	SPARA(j,2)	+	Settling speed of the sediment size. [L/T]
4	SPARA(j,3)	+	Critical shear stress for deposition of the sediment size. [M/L/T^2]
5	SPARA(j,4)	+	Critical shear stress for erosion of the j-th size fraction of sediment. [M/L/T^2]
6	SPARA(j,5)	+	Erodibility of the sediment size. [M/L^2]
7	SPARA(j,6)	+	Specific weight of the sediment size. [M/L^3]
8	SPARA(j,7)	+	Median diameter of particles in mixture of the sediment size. [L]
9	SPARA(j,8)	+	Critical bottom shear stress of the sediment size at which sediment movement begins. [M/L/T^2]

Field	Variable	Value	Description
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	3	Sorption rate constants and stoichiometry related to suspended sediment.
1	j	+	id of suspended sediment size.
2	i	+	id of dissolved chemical.
3	FKSPSS(j,1)	+	Forward rate constant of the sorption of i-th dissolved chemical onto the suspended sediment of the j-th size. [L^3/M/T]
4	BKSPSS(j,2)	+	Backward rate constant of the sorption of i-th dissolved chemical onto the suspended sediment of the j-th size. [1/T]

Field	Variable	Value	Description
C 1-2	IC1	ST	Card group identifier.
C 3	IC3	4	Sorption rate constants and stoichiometry related to bed sediment.
1	j	+	id of bed sediment size.
2	i	+	id of dissolved chemical.
3	FKSPBS(j,1)	+	Forward rate constant of the sorption of i-th dissolved chemical onto the bed sediment of the j-th size. [L^3/M/T]
4	BKSPBS(j,2)	+	Backward rate constant of the sorption of i-th dissolved chemical onto the bed sediment of the j-th size. [1/T]

VO card — Volatilization parameters

Field	Variable	Value	Description
C 1-2	IC1	VO	Card group identifier.
C 3	IC3	1	Volatilization rate constants.
1	j	+	id of dissolved chemical.
2	IAP(j)	+	id of xy series to describe the partial atmospheric pressure profile of the dissolved chemical. [atm]
3	FKVO(j)	+	Forward volatilization rate constant of the dissolved chemical. [1/T]
4	BKVO(j)	+	Backward volatilization rate constant of the dissolved chemical. [M/atm/L^3/T]

DY card — 1-st order decay parameters

Field	Variable	Value	Description
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	1	Decay constants of dissolved chemicals.
1	j	+	id of dissolved chemical.
2	DECAY(j)	+	1-st order decay constant of the dissolved chemical. [1/T]

Field	Variable	Value	Description
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	2	Decay constants of particulate chemicals on suspended sediments.
1	j	+	id of sediment size.
2	i	+	id of particulate chemical.
3	NCHEM	+	Number of dissolved chemicals.
4	DCY	+	Decay constant of the particulate chemical on the suspended sediment. [1/T]

Field	Variable	Value	Description
C 1-2	IC1	DY	Card group identifier.
C 3	IC3	3	Decay constants of particulate chemicals on bed sediments.
1	j	+	id of sediment size.
2	i	+	id of particulate chemical.
3	NCHEM	+	Number of dissolved chemicals.

4	NSSIZE	+	Number of sediment sizes.
5	DCY	+	Decay constant of the particulate chemical on the bed sediment. [1/T]

XY Card — X-Y Series Parameters

Field	Variable	Value	Description
C 1-2	IC1	XY	Card group identifier.
C 3	IC3	1	Generation of any x-y series function.
1	i	+	Index number for x-y series.
2	NPOINT(i)	+	The number of x-y values in the series.
3	DELTAX	0	Dummy values.
4	DELTAY	0	Dummy values.
5	REPEAT	0	Dummy values.
6	BEGCYC	0	Dummy values.
7	TNAME	+	A character string representing the name of the XY series.
(new line)X,Y			After XY card, the x-y values of the series are listed one pair per line up to NPOINT(i).

EN Card — End of data control

Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

1-D/2D Mapping File (.map files)

T1-T3 Cards — Job title
Only one T1, T2, and T3 card can be used.

CO Card — Mapping information

Field	Variable	Value	Description
C 1-2	IC1	CO	Card group identifier.
C 3	IC3	1	River/stream-related overland nodes
1	N	+	id of global river/stream node.
2	NP12(N)	+	id of the global overland node that is associated with the global river/stream node. This overland node will be excluded in overland simulations.
3	NPS12(1,N)	+	id of the global overland node that serves as the 1-st overland node next to the global river/stream node. This overland node is treated as a boundary node for overland simulations.
4	NPS12(2,N)	+	id of the global overland node that serves as the 2-nd overland node next to the global river/stream node. This overland node is treated as a boundary node for overland simulations.

EN Card — End of data control

Field	Variable	Value	Description
C1-2	IC1	EN	Card group identifier.
C 3	IC3	D	End of input data.

Table I.1 lists necessary parts for undergoing different simulations.

Table I.1 Data files required to achieve numerical simulations.

Simulations	Files required
1-D river/stream flow	Files 4 and 5
1-D river/stream transport	Files 4, 5, 6, and 7
1-D river/stream flow and transport	Files 4, 5, 6, and 7
2-D overland flow	Files 1 and 2
2-D overland transport	Files 1, 2, 3, and 7
2-D overland flow and transport	Files 1, 2, 3, and 7
1-D/2-D flow	Files 1, 2, 4, 5, and 8
1-D/2-D flow and transport	Files 1 through 8

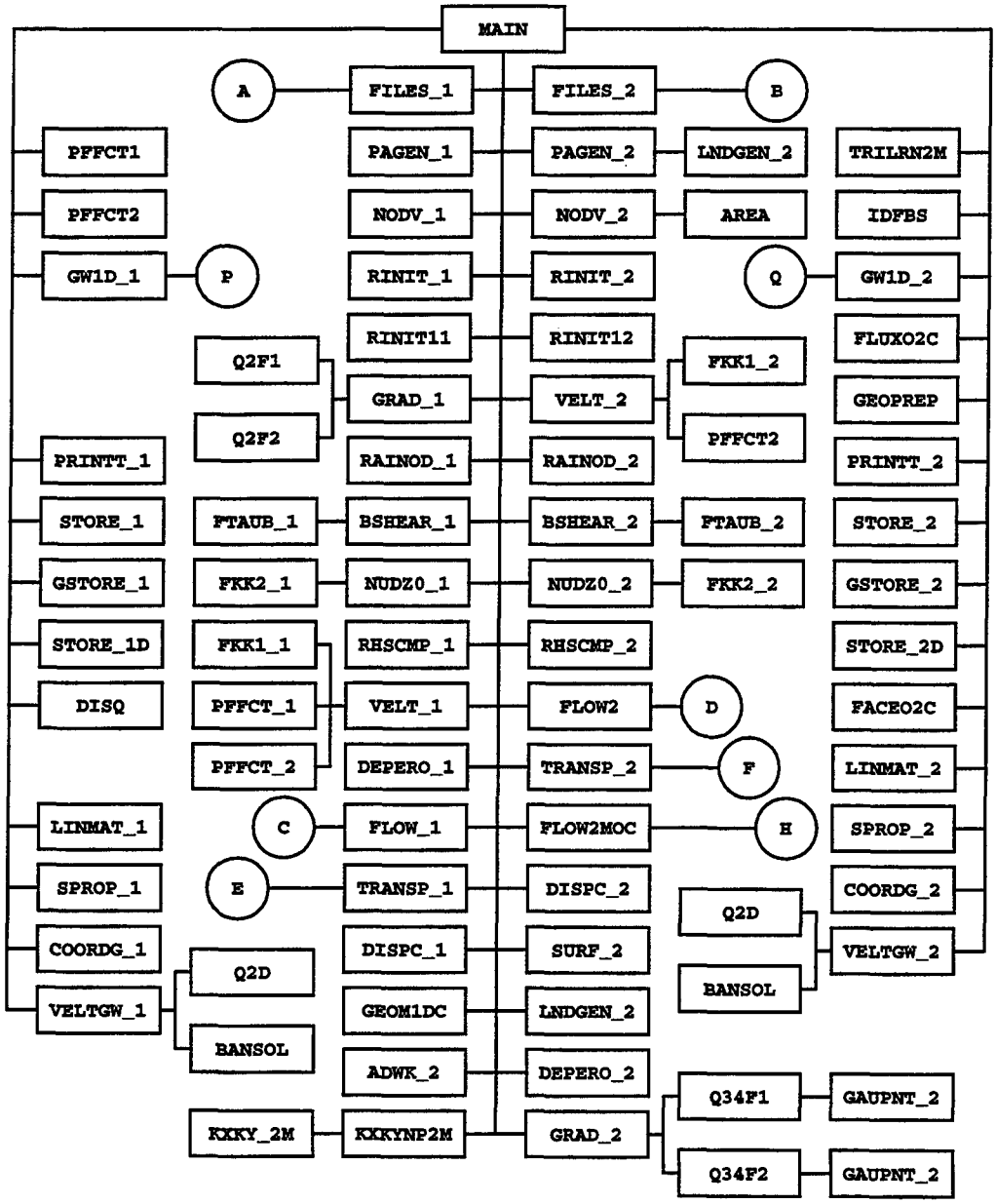
APPENDIX B PROGRAM STRUCTURE AND SUBROUTINE DESCRIPTION

In this appendix, we are to give plots showing the structure of the computer program and provide description for each subroutine.

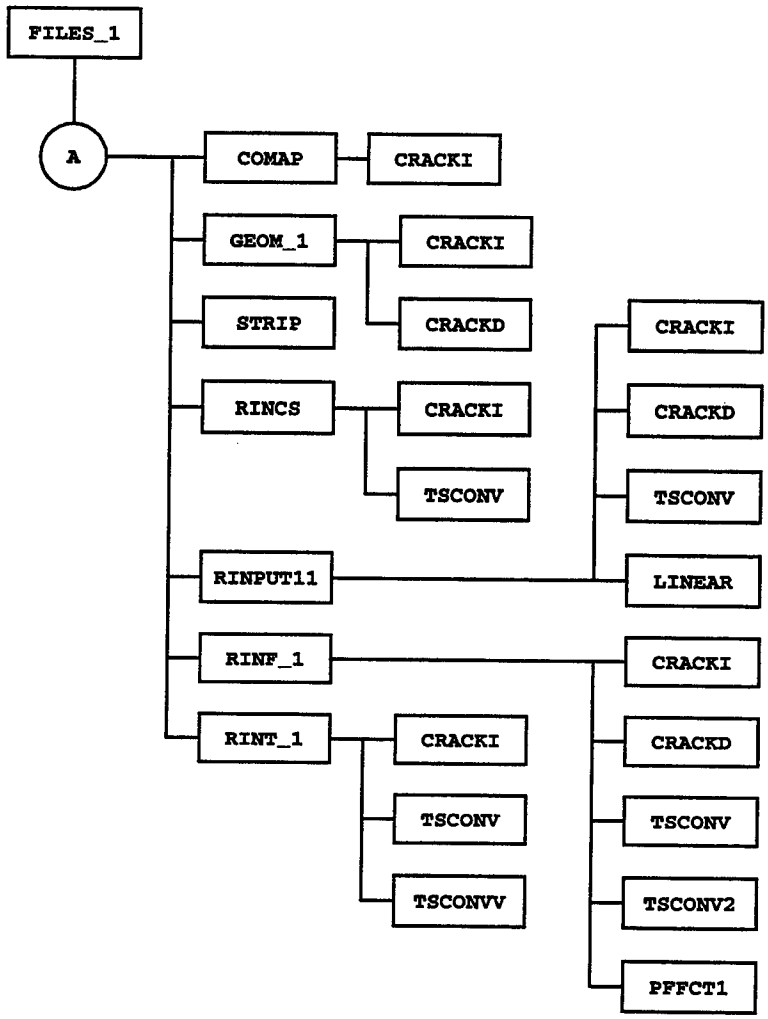
Program Structure

1

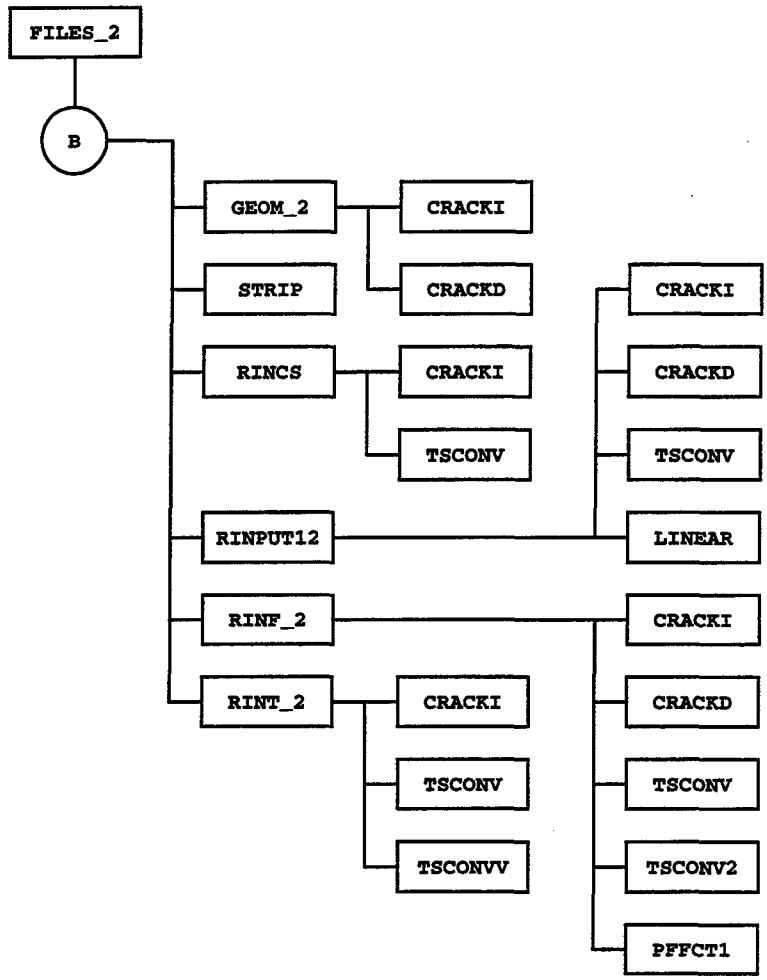
MAIN and the subroutines/functions it calls to.



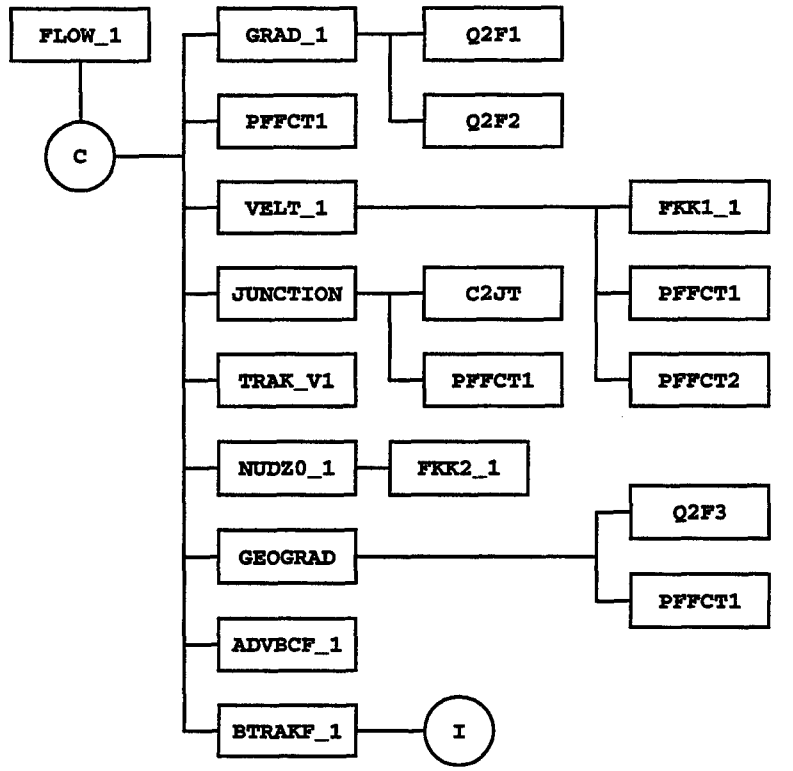
Subroutine FILES_1 and the subroutines/functions it calls to.



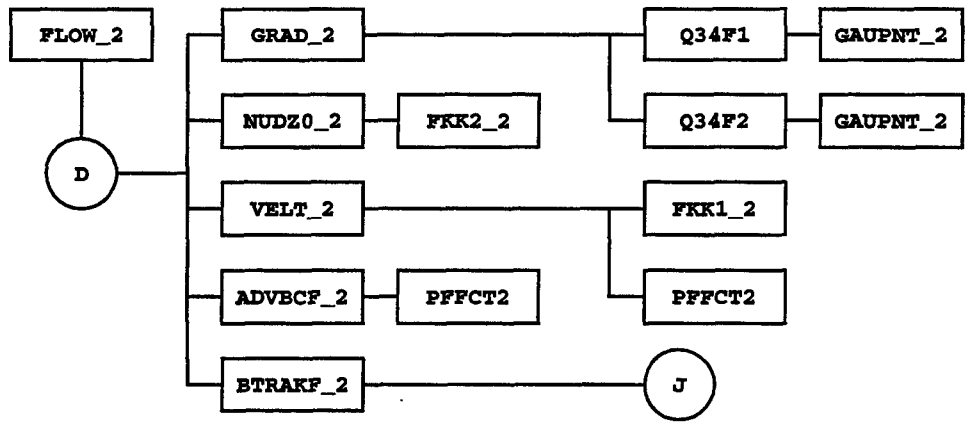
Subroutine FILES_2 and the subroutines/functions it calls to.



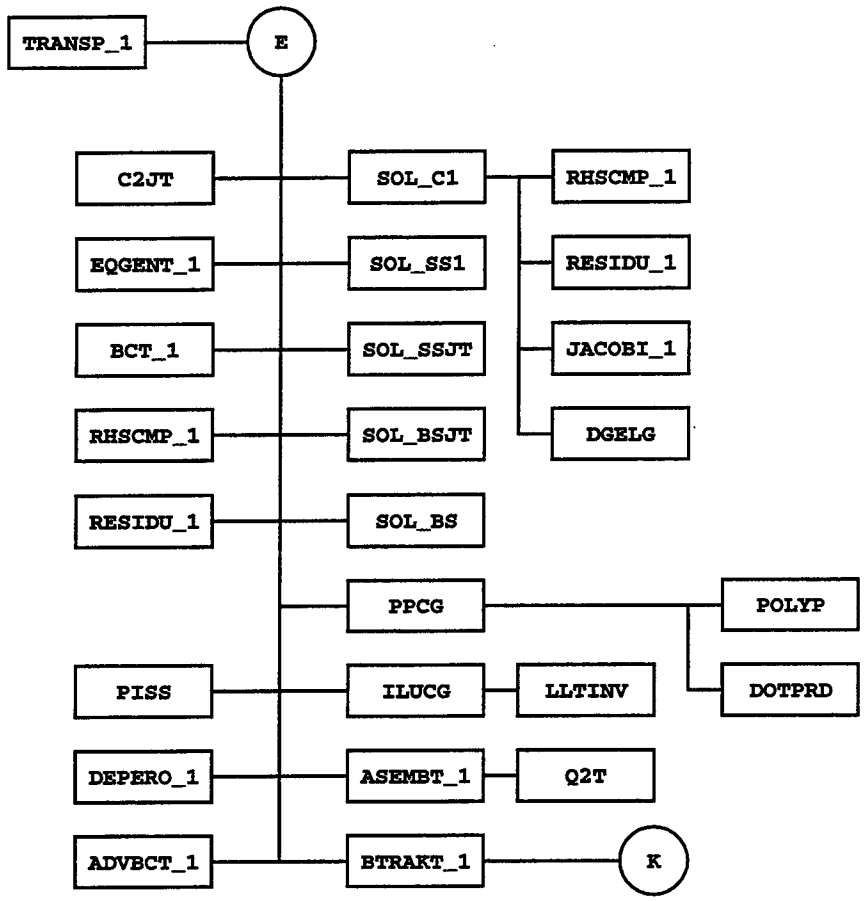
Subroutine FLOW_1 and the subroutines/functions it calls to.



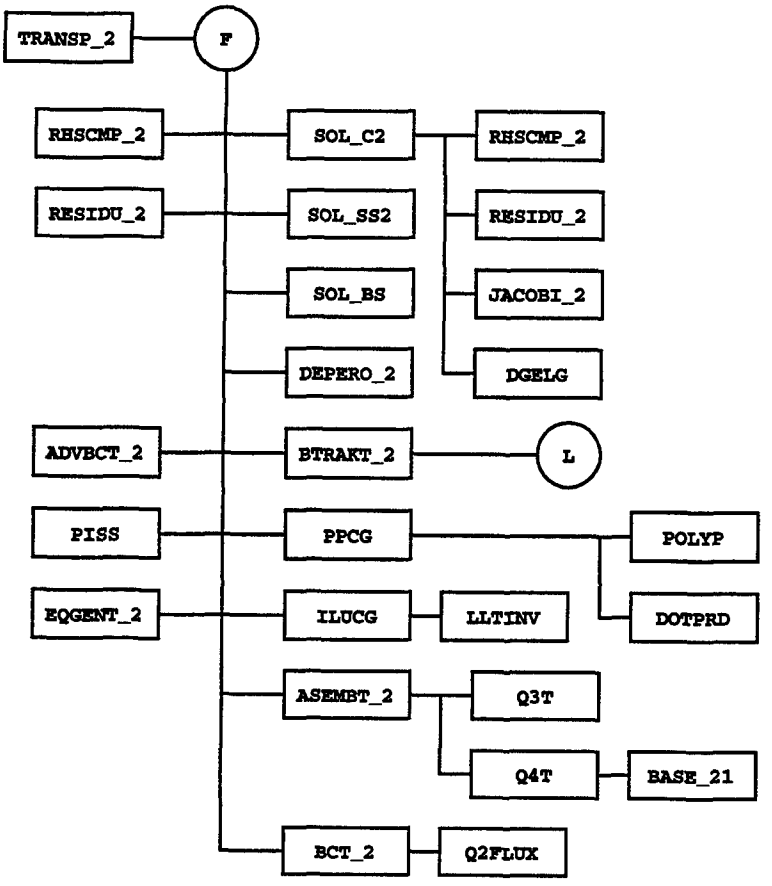
Subroutine FLOW_2 and the subroutines/functions it calls to.



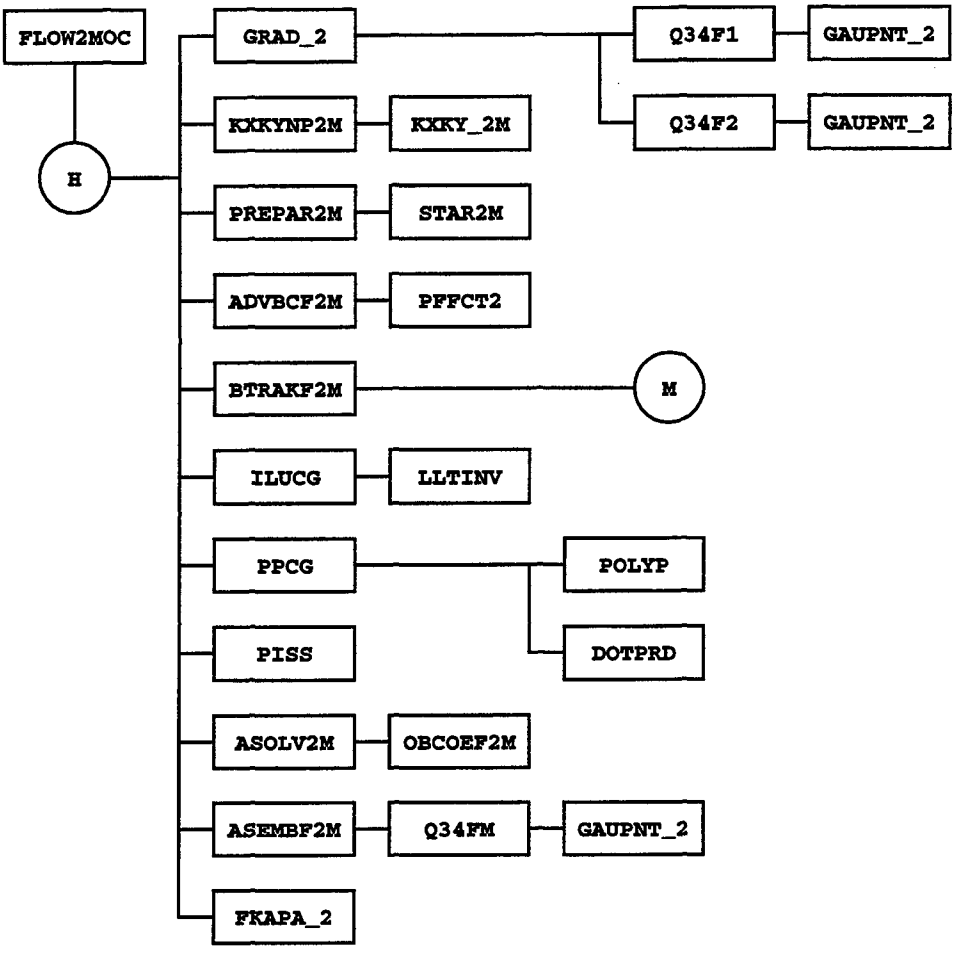
Subroutine TRANSP_1 and the subroutines/functions it calls.



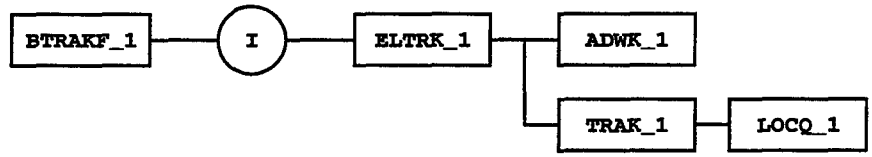
Subroutine TRANSP_2 and the subroutines/functions it calls to.



Subroutine FLOW2MOC and the subroutines/functions it calls.



Subroutine BTRAKF_1 and the subroutines/functions it calls to.



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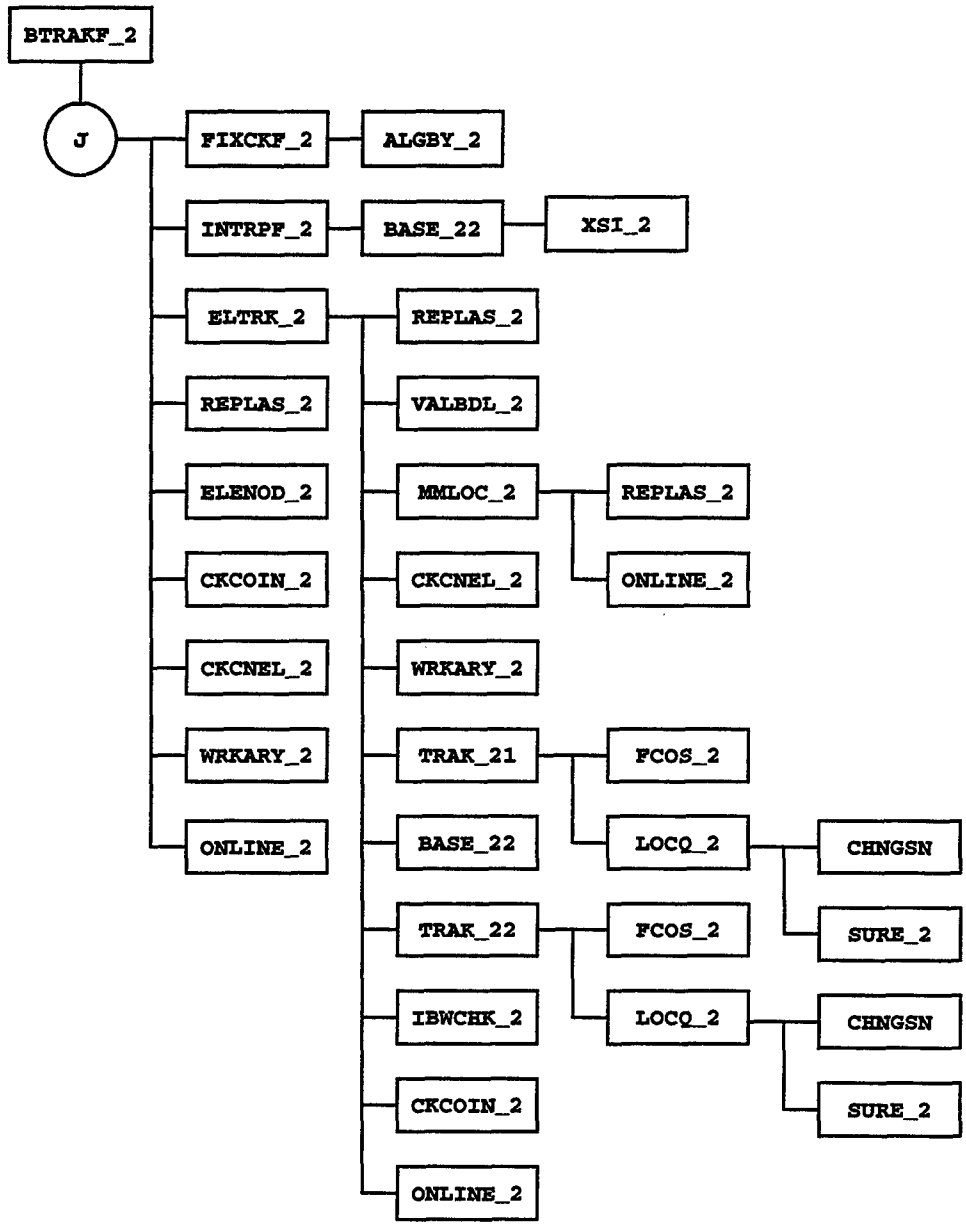
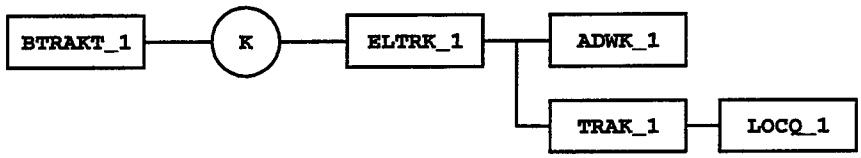
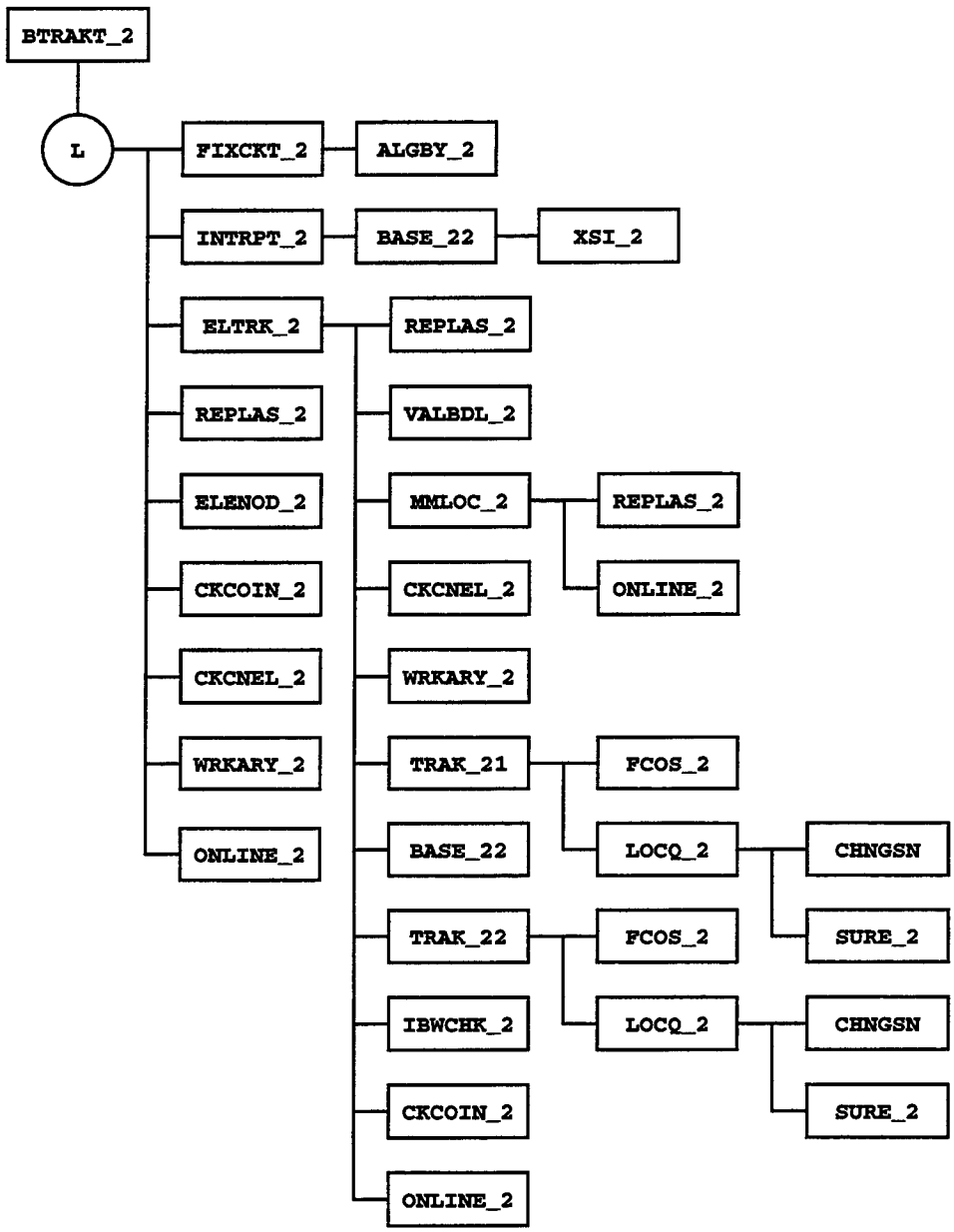
Subroutine BTRAKF_2 and the subroutines/functions it calls to.



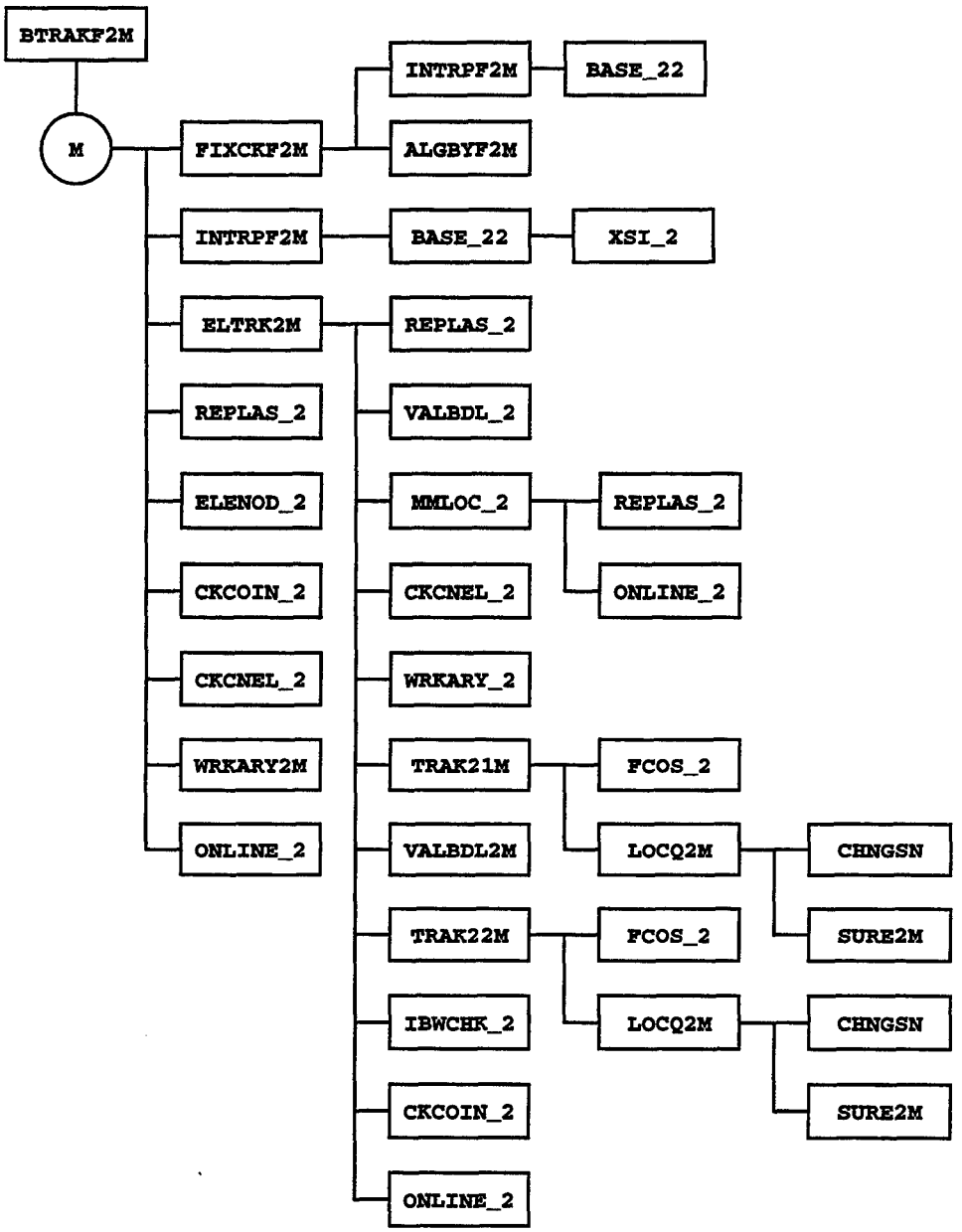
Subroutine BTRAKT_1 and the subroutines/functions it calls to.



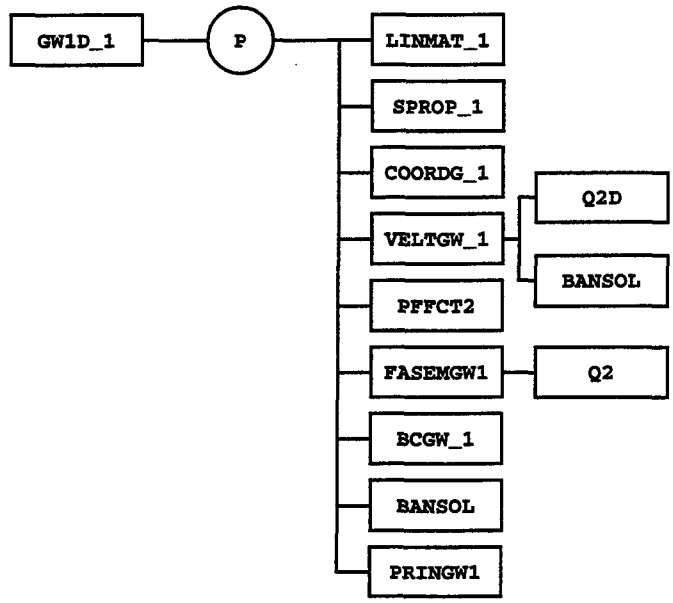
Subroutine BTRAKT_2 and the subroutines/functions it calls to.



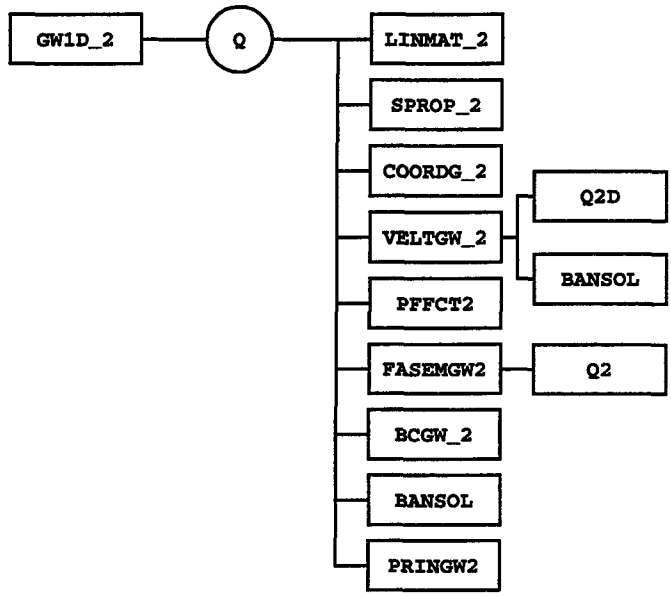
Subroutine BTRAKF2M and the subroutines/functions it calls to.



Subroutine GW1D_1 and the subroutines/functions it calls to.



Subroutine GW1D_2 and the subroutines/functions it calls to.



Subroutine Description

MAIN

This main program serves the purpose of controlling the flow path of desired simulations. It calls to Subroutines FILES_2 and FILES_1 to read in necessary data to undergo numerical simulations. It calls to Subroutines FLOW_2 or FLOW2MOC to compute 2-D overland flow, Subroutine TRANSP_2 to calculate 2-D overland transprot, Subroutine FLOW_1 to compute 1-D river/stream flow, and Subroutine TRANSP_1 to calculate 1-D river/stream transport. It also calls to Subroutine FLUXO2C to estimate both water and material flow rates from overland into river/stream, and vice versa. In addition, it calls to needed subroutines to print or store numerical results, including water depth, stage, discharge, velocity, and concentration, at desired times.

Subroutine ADVBCF_1

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 1-D flow equations. In this subroutine, boundary conditions with either water depth or upstream inflow specified are implemented to obtain water depth at associated boundary nodes. In addition, Dirichlet-type boundary conditions are applied to junction-connected river or stream nodes.

Subroutine ADVBCF_2

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 2-D flow equations. In this subroutine, boundary conditions with either water depth or upstream inflow specified are implemented to obtain water depth at associated boundary nodes. At the river/stream- and junction-related nodes, the flow direction is from river/stream or junction to the interior of overland, the flux is estimated and the corresponding water depth is calculated accordingly.

Subroutine ADVBCF2M

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 2-D flow equations when the method of characteristics is applied. In this subroutine, boundary conditions with either water stage or upstream inflow specified are implemented to obtain water stage or normal flux, respectively, at associated boundary nodes. At the river/stream- and junction-related nodes, the flow direction is from river/stream or junction to the interior of overland, the normal flux is estimated at the corresponding boundary nodes.

Subroutine ADVBCT_1

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 1-D transport equations of (1) suspended sediment, (2) dissolved chemicals, and (3) particulate chemicals on suspended sediments. Since the diffusive flux is neglected in the Lagrangian Step, only are the Dirichlet, Cauchy, and variable boundary conditions are applied. In

addition, Dirichlet-type boundary conditions are applied to junction-connected river/stream nodes.

Subroutine ADVBCT_2

This subroutine is to implement boundary conditions for the computation in the Lagrangian step of solving the 2-D transport equations of (1) suspended sediment, (2) dissolved chemicals, and (3) particulate chemicals on suspended sediments. Since the diffusive flux is neglected in the Lagrangian Step, only are the Dirichlet, Cauchy, and variable boundary conditions are applied. In addition, Variable-type boundary conditions are applied to river/stream- and junction-related overland nodes if flow direction is determined from river/stream/junction to overland.

Subroutine ADWK_1

This subroutine is to determine the working arrays of coordinates (XW) and velocities (VXW) in the element being considered in order to perform the 1-D "in-element" particle tracking.

Subroutine ADWK_2

This subroutine is to determine the working arrays of coordinates (XW), velocities (VXW), subelement indices (IEW), and element boundary index (IBW) in the element being considered in order to perform the 2-D "in-element" particle tracking.

Subroutine ALGBY_2

This subroutine is to achieve particle tracking along the 2-D unspecified boundary. Water flow is considered parallel to the boundary on the specified boundary. This subroutine also considers the first-order growth/decay term along characteristics.

Subroutine ALGBYF2M

This subroutine is to achieve particle tracking along the 2-D unspecified boundary. Water flow is considered parallel to the boundary on the specified boundary. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine AREA

This subroutine is to compute the area of a 2-D element.

Subroutine ASEMBF2M

This subroutine is to compose the global matrix equation to adjust 2-D velocity in the last part of the method of characteristic approach when eddy viscosity is taken into account.

Subroutine ASEMBT_1

This subroutine is to compute coefficient matrices CMATRX1 and CMATRX2 for 1-D transport equations. CMATRX1 is a mass matrice that takes into account the total time derivative term, while CMATRX2 is stiffness matrice that considers the dispersion term.

Subroutine ASEMBT_2

This subroutine is to compute coefficient matrices CMATRX1 and CMATRX2 for 2-D transport equations. CMATRX1 is a mass matrice that takes into account the total time derivative term, while CMATRX2 is stiffness matrice that considers the dispersion term.

Subroutine ASOLV2M

This subroutine is to construct and solve a set of three algebraic equations (Eqs. (3.133) through (3.135)) that is formed by using the method of characteristics to solve the dynamic wave model.

Subroutine BANSOL

This subroutine is to solver matrix equations with a direct band solver. When the first argument is set to 1, the subroutine triangularize the band coefficient matrice. When the argument is set to 2, the subroutine solves for the solution (back substitution).

Subroutine BASE_21

This subroutine is to compute the shape functions and their derivatives at a point located in a quadrilateral element, given the local coordinates at the point.

Subroutine BASE_22

This subroutine is to compute the shape functions at a point located in a 2-D element (either triangular or quadrilateral), given the Cartesian coordinates both at the point and element nodes.

Subroutine BCGW_1

This subroutine is to implement boundary conditions, including Cauchy, Neumann, and Dirichlet types, for the river/stream node-associated 1-D vertical subsurface flow.

Subroutine BCGW_2

This subroutine is to implement boundary conditions, including Cauchy, Neumann, and Dirichlet types, for the overland node-associated 1-D vertical subsurface flow.

Subroutine BCT_1

This subroutine is to implement boundary conditions, including Dirichlet, Cauchy, Neumann, conventional variable, and junction-related variable types, for 1-D river/stream transport. All boundary conditions, except for the junction-related variable type, are specified at boundary nodes (or reach ends) with time-dependent profiles. For junction-connected nodes, junction-related variable boundary conditions are applied.

Subroutine BCT_2

This subroutine is to implement boundary conditions, including Dirichlet, Cauchy, Neumann, conventional variable, and river/stream-related or junction-related variable types, for 2-D river or stream transport. Dirichlet boundary conditions are specified at boundary nodes, while the other types of boundary conditions are categorized as flux-type boundary conditions and are specified on boundary sides. Dirichlet, Cauchy, Neumann, and conventional variable boundary conditions are prescribed with time-dependent profiles, while river/stream- or junction-related variable boundary conditions are applied to their associated boundary sides.

Subroutine BSHEAR_1

This subroutine is to achieve the calculation of bottom shear stress at all river/stream nodes.

Subroutine BSHEAR_2

This subroutine is to achieve the calculation of bottom shear stress at all overland nodes.

Subroutine BTRAKF_1

This subroutine is implement backward particle tracking to obtain the water depth at all 1-D global nodes. Since a first-order approach is used for both kinematic and diffusion models and all source/sink rate terms can be expressed a linear function of water depth, we thus take into account the first-order decay/growth rate along the characteristics when we implement backward particle tracking. As for the zeroth-order source/sink rate, we simply multiply this rate by the time-step size being considered and add the product to the outcome of backward particle tracking.

Subroutine BTRAKF_2

This subroutine is implement backward particle tracking along three characteristics to obtain the Lagrangian water depth and veloctiy at all 2-D global nodes when the method of characteristics is used to solve 2-D flow equations. The spatial reachout approach is currently implemented in this subroutine.

Subroutine BTRAKF2M

This subroutine is implement backward particle tracking to obtain the water depth at all 2-D global nodes. Since a first-order approach is used for both kinematic and diffusion models and all

source/sink rate terms can be expressed a linear function of water depth, we thus take into account the first-order decay/growth rate along the characteristics when we implement backward particle tracking. As for the zeroth-order source/sink rate, we simply multiply this rate by the time-step size being considered and add the product to the outcome of backward particle tracking.

Subroutine BTRAKT_1

This subroutine is implement backward particle tracking to obtain the Lagrangian values of concentrations of (1) dissolved chemicals, (2) suspended sediments, and (3) particulate chemicals on suspended sediments at all 1-D global nodes.

Subroutine BTRAKT_2

This subroutine is implement backward particle tracking to obtain the Lagrangian values of concentrations of (1) dissolved chemicals, (2) suspended sediments, and (3) particulate chemicals on suspended sediments at all 2-D global nodes.

Subroutine CHNGSN

This subroutine is to change sign of the velocities at point P (the starting location), point Q (the ending location), and working subelement nodes in the process of 2-D or 3-D "in-element" particle tracking.

Subroutine CKCNEL_2

This subroutine is to determine the element that connects to a specified element through the element side with the N1-th and N2-th global nodes serving as the two end nodes of the side.

Subroutine CKCOIN_2

This subroutine is to determine whether or not a specific node coincides with the N1-th global node or the N2-th global node.

Subroutine COMAP

This subroutine is to relate 1-D river/stream nodes with 2-D overland nodes. Those overland nodes which correspond to river/stream nodes will not be taken into account in 2-D overland simulations.

Subroutine COORDG_1

This subroutine is to determine the coordinates of nodes for simulations of the river/stream node-associated 1-D vertical subsurface flow based on given specification.

Subroutine COORDG_2

This subroutine is to determine the coordinates of nodes for simulations of the overland node-associated 1-D vertical subsurface flow based on given specification.

Subroutine CRACKD

This subroutine is to read real numbers in order from a line data record.

Subroutine CRACKI

This subroutine is to read integer numbers in order from a line data record.

Subroutine C2JT

This subroutine is to compute the flow rate of (1) water (ID = 1), (2) dissolved chemicals (ID = 2), (3) particulate chemicals on suspended sediments (ID = 3), and (4) particulate chemicals on bed sediments (ID = 4) from junction-connected river/streams to a specified junction.

Subroutine DEPERO_1

This subroutine is to compute the deposition and erosion rates either at a river/stream node (when NP is not zero and J is zero) or at a junction (when NP equals zero and J is not equal to zero). Both cohesive and non-cohesive cases are taken into account. The following equations are used to achieve the computation at a river/stream node.

(1) For cohesive sediments:

$$D_n = V_{sn} S_n \left[1 - \frac{\tau_b}{\tau_{cDn}} \right] \qquad \text{(II.1)}$$

$$R_n = E_n \left[\frac{\tau_b}{\tau_{cRn}} - 1 \right] \qquad \text{(II.2)}$$

where V_{sn} is the settling velocity of the n-th size fraction sediment [L/T]; τ_b is the bottom shear stress or the bottom friction stress [M/L/T^2]; τ_{cDn} is the critical shear stress for the deposition of the n-th size fraction sediment [M/L/T^2]; τ_{cRn} is the critical shear stress for the erosion of the n-th size fraction sediment [M/L/T^2]; E_n is the erodibility of the n-th size fraction sediment [M/L^2]. In the computer code, V_{sn}, τ_{cDn}, τ_{cRn}, and E_n are input parameters, while τ_b is computed in the flow module.

(2) For non-cohesive sediments:

$$D_n = \frac{G_{sAn} - G_{sn}}{\Delta L} \qquad \text{(II.3)}$$

$$R_n = \frac{G_{sn} - G_{sAn}}{\Delta L} \tag{II.4}$$

where G_{sAn} is the actual load rate of the n-th size fraction sediment per unit width at a upstream location [M/L/T]; G_{sn} is the maximum load rate (capacity) of the n-th size fraction sediment per unit width at a downstream location [M/L/T]; ΔL is the distance between the upstream and the downstream locations. In the computer code, ΔL can be determined based on the coordinates, while G_{sAn} and G_{sn} are computed based on the following equations.

$$G_{sAn} = S_n * u * r \tag{II.5}$$

$$G_{sn} = 10 \frac{\rho^2 u\, r\, S\, (\tau_b - \tau_{crn})}{g\, d_n\, (\rho_{sn} - \rho)^2} \tag{II.6}$$

where ρ is the fluid density [M/L^3]; ρ_{sn} is the density of the n-th size fraction sediment [M/L^3]; u is river/stream flow velocity [L/T]; r is hydraulic radius [L]; S the friction slope, d_n is the median diameter of the n-th size fraction sediment particle [L]; g is gravity [L/T^2]; τ_{crn} is the critical bottom shear stress of the n-th size fraction sediment at which sediment movement begins [M/L/T^2]. Among these parameters, ρ, ρ_{sn}, d_n, and τ_{crn} are input by users, while u, r, and S are estimated in the flow module.

To estimate the deposition and erosion rates at a junction, the following weighted-average equations are employed.

$$D_n(J) = \frac{\sum_{i=1}^{NJRTH(J)} u_i P_i D_{ni}}{\sum_{i=1}^{NJRTH(J)} u_i P_i} \tag{II.7}$$

$$R_n(J) = \frac{\sum_{i=1}^{NJRTH(J)} u_i P_i R_{ni}}{\sum_{i=1}^{NJRTH(J)} u_i P_i} \tag{II.8}$$

where $D_n(J)$ and $R_n(j)$ are the deposition and erosion rate at the J-th junction; u_i, P_i, D_{ni}, R_{ni} are the velocity, wetted perimeter, deposition rate, and erosion rate at the river/stream node that serves as the i-th junction-connected node to the J-th junction; NJRTH(J) is number of river/stream reaches that are connected to the J-th junction.

Subroutine DEPERO_2

This subroutine is to compute the deposition and erosion rates at an overland node. The equations described in Subroutine DEPERO_1 are also used here.

Subroutine DGELG

This subroutine is to solve matrix equations by a direction solver incorporated with full-pivoting.

Subroutine DISPC_1

This subroutine is to compute dispersion coefficients for 1-D transport simulations. The coefficient is evaluated at every quadrature node of elements.

Subroutine DISPC_2

This subroutine is to compute dispersion coefficients for 2-D transport simulations. The coefficient is evaluated at every quadrature node of elements.

Subroutine DISQ

This subroutine is to compute discharge, based on the computed results, for printing or storing purposes.

Function DOTPRD

This function is to compute the inner product of two given vectors.

Subroutine ELENOD_2

This subroutine is to determine the number of element nodes for a specified element.

Subroutine ELTRK_1

This subroutine is to implement the 1-D "in-element" particle tracking for a particle with its starting location specified. During the tracking process, many elements can be passed through. The first-order growth/decay term is also taken into account in the tracking.

Subroutine ELTRK_2

This subroutine is to implement the 2-D "in-element" particle tracking in a specified element. The first-order growth/decay term is also taken into account in the tracking.

Subroutine ELTRK2M

This subroutine is to implement the 2-D "in-element" particle tracking in a specified element. It is used only when the method of characteristics is used to solve the 2-D flow equation.

Subroutine EQGENT_1

This subroutine is to generate matrix equations for 1-D transport simulations. When IDC = 0, it is for the transport of the IDS-th suspended sediment. When IDS = 0, it is for the transport of the IDC-th dissolved chemical. When neither IDC nor IDs equals zero, it is for the IDC-th particulate chemical on the IDS-th suspended sediment.

Subroutine EQGENT_2

This subroutine is to generate matrix equations for 2-D transport simulations. When IDC = 0, it is for the transport of the IDS-th suspended sediment. When IDS = 0, it is for the transport of the IDC-th dissolved chemical. When neither IDC nor IDs equals zero, it is for the IDC-th particulate chemical on the IDS-th suspended sediment.

Subroutine FACEO2C

This subroutine is to determine those overland boundary sides which are either river/stream-related or junction-related.

Subroutine FASEMGW1

This subroutine is to assemble matrix equations for computing the river/stream node-associated 1-D vertical subsurface flow.

Subroutine FASEMGW2

This subroutine is to assemble matrix equations for computing the overland node-associated 1-D vertical subsurface flow.

Function FCOS_2

This is to determine the direction of the outer product of two vectors.

Subroutine FILES_1

This subroutine is to read in information in order to perform 1-D river/stream simulations. The information includes (1) geometry data, (2) flow simulation data, and (3) transport simulation data.

Subroutine FILES_2

This subroutine is to read in information in order to perform 2-D river/stream simulations. The information includes (1) geometry data, (2) flow simulation data, and (3) transport simulation data.

Subroutine FIXCKF_2

This subroutine is to handle the case in the particle tracking of 2-D water flow when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolated is employed to compute the Lagrangian value. If this boundary is unspecified (closed), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached. The first-order growth/decay term is also taken into account in the tracking.

Subroutine FIXCKF2M

This subroutine is to handle the case in the particle tracking of 2-D water flow when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolated is employed to compute the Lagrangian value. If this boundary is unspecified (closed), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine FIXCKT_2

This subroutine is to handle the case in the particle tracking of 2-D chemical transport when a particle encounters the boundary. If this boundary is a specified (flow-through) boundary, the current particle tracking stops here and interpolated is employed to compute the Lagrangian value. If this boundary is unspecified (closed), on the other hand, the flow direction is parallel to the boundary and particle tracking along the boundary proceeds until either the available tracking time is completely consumed or a specified boundary is reached.

Function FKAPA_2

This function is to compute the bottom friction coefficient, κ, as defined as follows.

$$\kappa = \frac{gn\left|\nabla(h+Z_o)\right|^{1/2}\left[1+(\nabla Z_o)^2\right]^{2/3}}{h^{2/3}}$$

Subroutine FKK1_1

This subroutine is to compute the flow velocity at global nodes for either the kinematic model or the diffusion model of 1-D river/stream flow.

Subroutine FKK1_2

This subroutine is to compute the flow velocity at global nodes for either the kinematic model

or the diffusion model of 2-D overland flow.

Subroutine FKK2_1

This subroutine is to compute the source/sink term at a global node due to non-uniform bed slope or potential slope for the kinematic model or the diffusion model, respectively, of 1-D river/stream flow.

Subroutine FKK2_2

This subroutine is to compute the source/sink term at a global node due to non-uniform bed slope or potential slope for the kinematic model or the diffusion model, respectively, of 2-D overland flow.

Subroutine FLOW_1

This subroutine serves as the control panel of computing 1-D river/stream flow by using the Lagrangian approach to solve the diffusion model. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, the working velocity is first estimated based on the working water depth with Eq. (2.3). This working velocity is then used to achieve backward particle tracking in the Lagrangian approach to obtain the updated water depth. Convergence is determined by checking the maximum relative error of water depth. Relaxation technique is applied to update the working water depth for the next iteration if convergence has not been reached. When junctions exist, water budget is employed to determine the water depth at junctions. The flow rates of water coming from or going into the junction-connected reaches are calculated based on the working velocity and cross-sectional areas at junction-reach interfacial nodes (e.g., Nodes 10, 13, and 32 in Figure 4.4).

Subroutine FLOW_2

This subroutine serves as the control panel of computing 2-D overland flow by using the Lagrangian approach to solve the diffusion model. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, the working velocity is first estimated based on the working water depth with Eqs. (2.12) and (2.13). This working velocity is then used to achieve backward particle tracking in the Lagrangian approach to obtain the updated water depth. Convergence is determined by checking the maximum relative error or water depth. Relaxation technique is applied to update the working water depth for the next iteration if convergence has not been reached.

Subroutine FLOW2MOC

This subroutine serves as the control panel of computing 2-D overland flow by using the method of characteristics to solve the dynamic model. The Picard method is used to deal with nonlinearity. During each nonlinear iteration, The characteristic equations (Eq. (3.100)) are solved

first by the backward particle tracking along three characteristics. After $H^{\#}$, $u^{\#}$, and $v^{\#}$ are determined, we compute H, u, and v by solving Eqs. (3.147) through (3.149). Convergence is determined by checking the maximum relative error of H, u, and v. Relaxation technique is applied to update the working water stage and velocity for the next iteration if convergence has not been reached.

Subroutine FLUXO2C

This subroutine is to compute flow rate of water, dissolved chemicals, suspended sediments, and particulate chemicals on suspended sediments from overland to both river/stream nodes and river/stream junctions. When the outward normal velocity is positive at a river/stream- or junction-related overland boundary node, there is water flowing from overland to the associated river/stream node or junction. If the outward normal velocity is negative, two cases are taken into account: when the associated river/stream/junction water stage is higher than the bottom elevation of this overland boundary node, there is water flowing from river/stream/junction to overland: otherwise, there is no water passing through the 1D-2D interface.

Subroutine FTAUB_1

This subroutine is to calculate bottom shear stress at a river/stream node. The following equation is used to achieve the computation.

$$\tau = \rho g n r^{1/3} \left[1 + (\nabla Z_0)^2\right]^{2/3} \left|\nabla (h + Z_0)\right|^{1/2} u \qquad \text{(II.10)}$$

Subroutine FTAUB_2

This subroutine is to calculate bottom shear stress at an overland node. The following equations are used to achieve the computation.

$$\tau_x = \rho g n h^{1/3} \left[1 + (\nabla Z_0)^2\right]^{2/3} \left|\nabla (h + Z_0)\right|^{1/2} u \qquad \text{(II.11)}$$

$$\tau_y = \rho g n h^{1/3} \left[1 + (\nabla Z_0)^2\right]^{2/3} \left|\nabla (h + Z_0)\right|^{1/2} v \qquad \text{(II.12)}$$

Subroutine GAUPNT_2

This subroutine is to compute shape functions and their derivatives at quadrature nodes.

Subroutine GEOGRAD

This subroutine is to compute the derivatives of hydraulic radius and average river/stream width with respect to distance and water depth in 1-D river/stream flow simulations.

Subroutine GEOM1DC

This subroutine is to determine the river/stream-associated overland elements that are not to

be taken into account in 2-D overland simulations.

Subroutine GEOM_1

This subroutine is to read in 1-D river/stream geometry, including coordinates and element indices.

Subroutine GEOM_2

This subroutine is to read in 2-D overland geometry, including coordinates and element indices.

Subroutine GEOPREP

This subroutine is to prepare the profile of describing the derivatives of both hydraulic radius and average river/stream width with respect to water depth, based on the prescribed profiles of river/stream geometry.

Subroutine GRAD_1

This subroutine is to compute the spatial derivatives of water depth, stage, flow velocity, average river/stream width, and Manning's n as desired in 1-D river/stream simulations. In addition, the second spatial derivatives of water depth and stage are calculated as needed.

Subroutine GRAD_2

This subroutine is to compute the spatial derivatives of water depth, stage, flow velocity, and Manning's n as desired in 2-D overland simulations. In addition, the second spatial derivatives of water depth and stage are calculated as needed.

Subroutine GSTORE_1

This subroutine is to store pertinent quantities for post-processing of 1-D river/stream simulations.

Subroutine GSTORE_2

This subroutine is to store pertinent quantities for post-processing of 2-D overland simulations.

Subroutine GW1D_1

This subroutine is to control the flow of computing the 1-D vertical subsurface flow that is associated with each river/stream node.

Subroutine GW1D_2

This subroutine is to control the flow of computing the 1-D vertical subsurface flow that is associated with each overland node.

Subroutine IBWCHK_2

This subroutine is to determine the two global nodes that serve as the two end node of an element side. This element side is the side that the particle has encountered when it passes through the element being considered.

Subroutine IDFBS

This subroutine is to relate flux-type boundary sides with global boundary sides. The relationship is stored in two arrays: one for flow simulations and the other for transport simulations.

Subroutine ILUCG

This subroutine is to solve the linearized matrix equation that is sparse asymmetric with the preconditioned conjugate gradient method using the incomplete Cholesky decomposition as a preconditioner.

Subroutine INTRPF_2

This subroutine is to determine the Lagrangian water depth by interpolation after backward particle tracking in solving flow governing equations

Subroutine INTRPF2M

Subroutine INTRPT_2

This subroutine is to determine the Lagrangian chemical and suspended sediment concentrations by interpolation after backward particle tracking in the Lagrangian step of solving transport governing equations

Subroutine JACOBI_1

This subroutine is to compute the Jacobian for the chemical system at the NP-th node (when NP is not equal to zero and J equals zero) or the J-th junction (when NP equals zero and J is not equal to zero). The Jacobian elements are defined as follows.

<u>For the case at the NP-th node:</u>

(1) For dissolved chemicals:

$$\frac{\partial RESC_i}{\partial (C_l^{\,w})^{N+1}} = \delta_{il} A + \delta_{il}\,\delta t \left[\lambda_i^{w} A + R - I + R_1 + R_2 + A k_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} \right] -$$

$$\delta t \left[\sum_{m=1}^{N_{rx}} k_m^{rb} A b_{ml} (C_l^{\,w})^{b_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{\,w})^{b_{mj}} - \sum_{m=1}^{N_{rx}} k_m^{rf} A a_{ml} (C_l^{\,w})^{a_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{\,w})^{a_{mj}} \right] \qquad \text{(II.13)}$$

$$i \in [1, N_c]$$

$$\frac{\partial RESC_i}{\partial (C_{nl}^{\,s})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sb} S_n A \qquad n \in [1, N_s],\quad i \in [1, N_c], \qquad \text{(II.14)}$$

$$\frac{\partial RESC_i}{\partial (C_{nl}^{\,b})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{bb} M_n P \qquad n \in [1, N_s],\quad i \in [1, N_c] \qquad \text{(II.15)}$$

(2) For particulate chemicals on suspended sediments:

$$\frac{\partial RESC_k}{\partial (C_l^{\,w})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sf} S_n A \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = n * N_c + i \qquad \text{(II.16)}$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{\,s})^{N+1}} = \delta_{il} A S_n + \delta_{il}\,\delta t\, B D_n + \delta_{il}\,\delta t\, S_n \left[\lambda_{ni}^{s} A + k_{ni}^{sb} A + R - I + R_1 + R_2 \right] \qquad \text{(II.17)}$$

$$n \in [1, N_s],\quad i \in [1, N_c],\quad k = n * N_c + i$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{\,b})^{N+1}} = -\delta_{il}\,\delta t\, B R_n \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = n * N_c + i \qquad \text{(II.18)}$$

(3) For particulate chemicals on bed sediments:

$$\frac{\partial RESC_k}{\partial (C_l^{\,w})^{N+1}} = -\delta_{il}\,\Delta t\, k_{ni}^{bf} M_n \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = (n + N_s) * N_c + i \qquad \text{(II.19)}$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{\,s})^{N+1}} = -\delta_{il}\,\Delta t\, D_n \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = (n + N_s) * N_c + i \qquad \text{(II.20)}$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{\,b})^{N+1}} = \delta_{il} M_n + \delta_{il}\,\Delta t\, R_n + \delta_{il}\,\Delta t\, M_n \left[\lambda_{ni}^{b} + k_{ni}^{bb} \right] \qquad \text{(II.21)}$$

$$n \in [1, N_s],\quad i \in [1, N_c],\quad k = (n + N_s) * N_c + i$$

<u>For the case at the J-th junction:</u>

(1) For dissolved chemicals:

$$\frac{\partial RESC_i}{\partial (C_l^{w}(J))^{N+1}} = \delta_{il} V(J) + \delta_{il} \Delta t \left[\lambda_i^{w} V(J) + V(J) k_i^{af} + \sum_{n=1}^{N_s} S_n(J) V(J) k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n(J) A(J) k_{ni}^{bf} \right] -$$

$$\Delta t \left[\sum_{m=1}^{N_{rx}} k_m^{rb} V(J) b_{ml} (C_l^{w}(J))^{b_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{w}(J))^{b_{mj}} - \sum_{m=1}^{N_{rx}} k_m^{rf} V(J) a_{ml} (C_l^{w}(J))^{a_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{w}(J))^{a_{mj}} \right] \quad \text{(II.22)}$$

$$i \in [1, N_c]$$

$$\frac{\partial RESC_i}{\partial (C_{nl}^{s}(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{sb} S_n(J) V(J) \qquad n \in [1, N_s], \quad i \in [1, N_c], \quad \text{(II.23)}$$

$$\frac{\partial RESC_i}{\partial (C_{nl}^{b}(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bb} M_n(J) A(J) \qquad n \in [1, N_s], \quad i \in [1, N_c] \quad \text{(II.24)}$$

(2) For particulate chemicals on suspended sediments:

$$\frac{\partial RESC_k}{\partial (C_l^{w}(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{sf} S_n(J) V(J) \qquad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad \text{(II.25)}$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{s}(J))^{N+1}} = \delta_{il} V(J) S_n(J) + \delta_{il} \Delta t A(J) D_n(J) + \delta_{il} \Delta t S_n(J) \left[\lambda_{ni}^{s} V(J) + k_{ni}^{sb} V(J) \right] \quad \text{(II.26)}$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{b}(J))^{N+1}} = -\delta_{il} \Delta t A(J) R_n(J) \qquad n \in [1, N_s], \quad i \in [1, N_c], \quad k = n * N_c + i \quad \text{(II.27)}$$

(3) For particulate chemicals on bed sediments:

$$\frac{\partial RESC_k}{\partial (C_l^{w}(J))^{N+1}} = -\delta_{il} \Delta t k_{ni}^{bf} M_n(J) \qquad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad \text{(II.28)}$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{s}(J))^{N+1}} = -\delta_{il} \Delta t D_n(J) \qquad n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i \quad \text{(II.29)}$$

$$\frac{\partial RESC_k}{\partial (C_{nl}^{b}(J))^{N+1}} = \delta_{il} M_n(J) + \delta_{il} \Delta t R_n(J) + \delta_{il} \Delta t M_n(J) \left[\lambda_{ni}^{b} + k_{ni}^{bb} \right] \quad \text{(II.30)}$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

Subroutine JACOBI_2

This subroutine is to compute the Jacobian for the chemical system at the NP-th node. The Jacobian elements are defined as follows.

(1) For dissolved chemicals:

$$\frac{\partial RES(i)}{\partial (C_l^{\,w})^{N+1}} = \delta_{il} h + \delta_{il}\,\delta t \left[\lambda_i^w h + R - I + h k_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} \right] -$$

$$\delta t \left[\sum_{m=1}^{N_{r\alpha}} k_m^{rb} h b_{ml} (C_l^{\,w})^{b_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{\,w})^{b_{mj}} - \sum_{m=1}^{N_{r\alpha}} k_m^{rf} h a_{ml} (C_l^{\,w})^{a_{ml}-1} \prod_{j=1, j\neq l}^{N_c} (C_j^{\,w})^{a_{mj}} \right] \qquad \text{(II.31)}$$

$$i \in [1, N_c]$$

$$\frac{\partial RES(i)}{\partial (C_{nl}^{\,s})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sb} S_n h \qquad n \in [1, N_s],\quad i \in [1, N_c], \qquad \text{(II.32)}$$

$$\frac{\partial RES(i)}{\partial (C_{nl}^{\,b})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{bb} M_n \qquad n \in [1, N_s],\quad i \in [1, N_c] \qquad \text{(II.33)}$$

(2) For particulate chemicals on suspended sediments:

$$\frac{\partial RES(k)}{\partial (C_l^{\,w})^{N+1}} = -\delta_{il}\,\delta t\, k_{ni}^{sf} S_n h \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = n * N_c + i \qquad \text{(II.34)}$$

$$\frac{\partial RES(k)}{\partial (C_{nl}^{\,s})^{N+1}} = \delta_{il} h S_n + \delta_{il}\,\delta t\, D_n + \delta_{il}\,\delta t\, S_n \left[\lambda_{ni}^s h + k_{ni}^{sb} h + R - I \right]$$

$$n \in [1, N_s],\quad i \in [1, N_c],\quad k = n * N_c + i \qquad \text{(II.35)}$$

$$\frac{\partial RES(k)}{\partial (C_{nl}^{\,b})^{N+1}} = -\delta_{il}\,\delta t\, R_n \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = n * N_c + i \qquad \text{(II.36)}$$

(3) For particulate chemicals on bed sediments:

$$\frac{\partial RES(k)}{\partial (C_l^{\,w})^{N+1}} = -\delta_{il}\,\Delta t\, k_{ni}^{bf} M_n \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = (n + N_s) * N_c + i \qquad \text{(II.37)}$$

$$\frac{\partial RES(k)}{\partial (C_{nl}^{\,s})^{N+1}} = -\delta_{il}\,\Delta t\, D_n \qquad n \in [1, N_s],\quad i \in [1, N_c],\quad k = (n + N_s) * N_c + i \qquad \text{(II.38)}$$

$$\frac{\partial RES(k)}{\partial (C_{nl}^{b})^{N+1}} = \delta_{il} M_n + \delta_{il} \Delta t R_n + \delta_{il} \Delta t M_n \left[\lambda_{ni}^{b} + k_{ni}^{bb} \right] \qquad \text{(II.39)}$$

$$n \in [1, N_s], \quad i \in [1, N_c], \quad k = (n + N_s) * N_c + i$$

Subroutine JUNCTION

This subroutine is to update water depths (stages) at junctions based on the concept of water budget.

Subroutine KXKY_2M

This subroutine is to determine characteristic directions at a 2-D global node for overland flow simulations, based on the velocity, the spatial velocity derivatives, and the spatial stage derivatives at the node. This subroutine is needed only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine KXKYNP2M

This subroutine is to determine characteristic directions at all 2-D global nodes for overland flow simulations. This subroutine is needed only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine LINEAR

This subroutine is to determine a functional value through linear interpolation.

Subroutine LINMAT_1

This subroutine is to record material types along the 1-D vertical lines that are associated with 1-D river/stream nodes.

Subroutine LINMAT_2

This subroutine is to record material types along the 1-D vertical lines that are associated with 2-D overland nodes.

Subroutine LLTINV

This subroutine is to solve for a modified residual that is to be used in the preconditioned conjugate gradient algorithm.

Subroutine LNDGEN_2

This subroutine is to determine node-node and node-element connectivity in 2-D simulations, based on the given element indices.

Subroutine LOCQ_1

This subroutine is to locate the target point and its velocity for a tracking path in a 1-D subelement of particle tracking.

Subroutine LOCQ_2

This subroutine is to locate the target point and its velocity for a tracking path in a 2-D subelement of particle tracking. The available tracking time left after this tracking path is also computed.

Subroutine LOCQ2M

This subroutine is to locate the target point and its velocity for a tracking path in a 2-D subelement of particle tracking. The available tracking time left after this tracking path is also computed. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine MMLOC_2

This subroutine is to specify the starting location to start the 2-D "in-element" particle tracking in an element. The available tracking time left after this tracking path is also computed.

Subroutine NODV_1

This subroutine is to calculate Manning's n at every 1-D global node.

Subroutine NODV_2

This subroutine is to calculate Manning's n at every 2-D global node.

Subroutine NUDZ0_1

This subroutine is to compute the source term, which is coming from non-uniform bed slopes (in the case of kinematic model) or potential slope (in the case of diffusive model), for all global nodes in 1-D river/stream flow simulations.

Subroutine NUDZ0_2

This subroutine is to compute the source term, which is coming from non-uniform bed slopes (in the case of kinematic model) or potential slope (in the case of diffusive model), for all global

nodes in 2-D overland flow simulations.

Subroutine OBCOEF2M

This subroutine is to determine the coefficient of a characteristic at an open boundary node. The characteristic has been determined coming from the outside of the domain.

Subroutine ONLINE_2

This subroutine is to adjust the coordinates of a specified point if needed, such that this point will be located on the line segment with two given nodes serving as its end nodes.

Subroutine PAGEN_1

This subroutine is to generate 1-D pointer arrays needed for numerical simulations.

Subroutine PAGEN_2

This subroutine is to generate 2-D pointer arrays needed for numerical simulations.

Subroutine PFFCT1

This subroutine is to determine the functional value by interpolation from a given profile.

Subroutine PFFCT2

This subroutine is to determine the functional values of an array by interpolation from a series of given profiles.

Subroutine PISS

This subroutine is to solver the linearized matrix equation with a pointwise iteration solution strategy.

Subroutine POLYP

This subroutine is to solve a modified residual that is to be used in the preconditioned conjugate gradient algorithm.

Subroutine PPCG

This subroutine is to solve the linearized matrix equation with the preconditioned conjugate gradient method by using a polynomial as a preconditioner.

Subroutine PREPAR2M

This subroutine is to prepare for data needed to construct and solve the set of algebraic equations in Subroutine ASOLV2M.

Subroutine PRINGW1

This subroutine is to write out simulation results of the 1-D vertical subsurface flow simulations that are corresponding to river/stream nodes.

Subroutine PRINGW2

This subroutine is to write out simulation results of the 1-D vertical subsurface flow simulations that are corresponding to overland nodes.

Subroutine PRINTT_1

This subroutine is to write out simulation results of 1-D river/stream simulations.

Subroutine PRINTT_2

This subroutine is to write out simulation results of 2-D overland simulations.

Subroutine Q2

This subroutine is to estimate the integration over a line element.

Subroutine Q2D

This subroutine is to estimate the integration over a line element.

Subroutine Q2FLUX

This subroutine is to perform boundary integration over a 2-D boundary side.

Subroutine Q2F1

This subroutine is to determine element coefficient matrices and load vector to compute the gradients of bottom elevation, water stage, velocities, and Manning's n in 1-D river/stream flow simulations.

Subroutine Q2F2

This subroutine is to determine element coefficient matrices and load vector to compute the gradients of the derivatives of bottom elevation in 1-D river/stream flow simulations.

Subroutine Q2F3

This subroutine is to determine element coefficient matrices and load vector to compute the gradients of hydraulic radius and average river/stream width in 1-D river/stream flow simulations.

Subroutine Q2T

This subroutine is to determine the line element coefficient matrices and load vector to sole 1-D transport equation in the Eulerian step.

Subroutine Q3T

This subroutine is to determine the triangular element coefficient matrices and load vector to sole 2-D transport equation in the Eulerian step.

Subroutine Q4T

This subroutine is to determine the quadrilateral element coefficient matrices and load vector to sole 2-D transport equation in the Eulerian step.

Subroutine Q34FM

This subroutine is to determine the element coefficient matrices, including mass matrices and the stiffness matrices taking into account eddy viscosity in soling 2-D dynamic wave model.

Subroutine Q34F1

This subroutine is to determine element coefficient matrices and load vector to compute the gradients of bottom elevation, water stage, velocities, and Manning's n in 2-D overland flow simulations.

Subroutine Q34F2

This subroutine is to determine element coefficient matrices and load vector to compute the gradients of the derivatives of bottom elevation in 2-D overland flow simulations.

Subroutine RAINOD_1

This subroutine is to determine rainfall rate at 1-D global nodes.

Subroutine RAINOD_2

This subroutine is to determine rainfall rate at 2-D global nodes.

Subroutine REPLAS_2

This subroutine is to write the values of the first four arguments into the last four arguments.

Subroutine RESIDU_1

This subroutine is compute the residual of the 1-D transport equations of (1) dissolved chemicals (ID = 1), (2) particulate chemicals on suspended sediments (ID = 1), (3) particulate chemicals on bed sediments (ID = 1), and (4) suspended sediments (ID = 2) at the NP-th node (when NP is not equal to zero and J equals zero) or the J-th junction (when NP equals zero and J is not equal to zero). The residuals are defined as follows.

<u>For the case at the NP-th node:</u>

(1) For dissolved chemicals:

$$RESC_i = A\left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2}\right] - \delta t\,(RHSC_i)^{N+1} + \delta t\,(RHSC_i)^N \qquad i \in [1,N_c] \qquad \text{(II.40)}$$

(2) For particulate chemicals on suspended sediments:

$$RESC_k = A\left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}\right] - \delta t\,(RHSC_k)^{N+1} + \delta t\,(RHSC_k)^N$$
$$n \in [1,N_s], \quad i \in [1,N_c], \quad k = n * N_c + i \qquad \text{(II.41)}$$

(3) For particulate chemicals on bed sediments:

$$RESC_k = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t\,(RHSC_k)^{N+1}$$
$$n \in [1,N_s], \quad i \in [1,N_c], \quad k = (n + N_s) * N_c + i \qquad \text{(II.42)}$$

(4) For suspended sediments:

$$RESS_n = A(S_n)^{N+1/2} + \delta t\,(RHSS_n)^{N+1} - \delta t\,(RHSS_n)^N \qquad n \in [1,N_s] \qquad \text{(II.43)}$$

where $(RHSS_n)^{N+1}$ is evaluated with ID = 22 in subroutine RHSCOMP1, whereas $(RHSS_n^N)$ is calculated with ID = 21.

<u>For the case at the J-th junction:</u>

(1) For dissolved chemicals:

$$RESC_i = \left[(V(J)C_i^w(J))^{N+1} - (V(J)C_i^w(J))^N\right] - \Delta t\,(RHSC_i)^{N+1} \qquad i \in [1,N_c] \qquad \text{(II.44)}$$

(2) For particulate chemicals on suspended sediments:

$$RESC_k = \left[(V(J)S_n(J)C_{ni}^s(J))^{N+1} - (V(J)S_n(J)C_{ni}^s(J))^N\right] - \Delta t\,(RHSC_k)^{N+1}$$
$$n \in [1,N_s], \quad i \in [1,N_c], \quad k = n * N_c + i \qquad \text{(II.45)}$$

(3) For particulate chemicals on bed sediments:

$$RESC_k = (M_n(J)C_{ni}^b(J))^{N+1} - (M_n(J)C_{ni}^b(J))^N - \Delta t\,(RHSC_k)^{N+1}$$
$$n\in[1,N_s],\quad i\in[1,N_c],\quad k=(n+N_s)*N_c+i \qquad \text{(II.46)}$$

(4) For suspended sediments:

$$RESS_n = (V(J)S_n(J))^N + \Delta t\,(RHSS_n)^{N+1} \qquad n\in[1,N_s] \qquad \text{(II.47)}$$

Subroutine RESIDU_2

This subroutine is compute the residual of the 2-D transport equations of (1) dissolved chemicals (ID = 1), (2) particulate chemicals on suspended sediments (ID = 1), (3) particulate chemicals on bed sediments (ID = 1), and (4) suspended sediments (ID = 2) at the NP-th node. The residuals are defined as follows

For the case at the NP-th node:

(1) For dissolved chemicals:

$$RESC_i = h\left[(C_i^w)^{N+1} - (C_i^w)^{N+1/2}\right] - \delta t\,(RHSC_i)^{N+1} + \delta t\,(RHSC_i)^N \qquad i\in[1,N_c] \qquad \text{(II.48)}$$

(2) For particulate chemicals on suspended sediments:

$$RESC_k = h\left[(S_n C_{ni}^s)^{N+1} - (S_n C_{ni}^s)^{N+1/2}\right] - \delta t\,(RHSC_k)^{N+1} + \delta t\,(RHSC_k)^N$$
$$n\in[1,N_s],\quad i\in[1,N_c],\quad k=n*N_c+i \qquad \text{(II.49)}$$

(3) For particulate chemicals on bed sediments:

$$RESC_k = (M_n C_{ni}^b)^{N+1} - (M_n C_{ni}^b)^N - \Delta t\,(RHSC_k)^{N+1}$$
$$n\in[1,N_s],\quad i\in[1,N_c],\quad k=(n+N_s)*N_c+i \qquad \text{(II.50)}$$

(4) For suspended sediments:

$$RESS_n = h(S_n)^{N+1/2} + \delta t\,(RHSS_n)^{N+1} - \delta t\,(RHSS_n)^N \qquad n\in[1,N_s] \qquad \text{(II.51)}$$

where $(RHSS_n)^{N+1}$ is evaluated with ID = 22 in subroutine RHSCOMP1, whereas $(RHSS_n^N)$ is calculated with ID = 21.

Subroutine RHSCMP_1

This subroutine is to compute the right-hand side of the 1-D transport governing equations of (1) dissolved chemicals (ID = 1), (2) particulate chemicals on suspended sediments (ID = 1), (3) particulate chemicals on bed sediments (ID = 1), and (4) suspended sediments (ID = 21 or 22) at the NP-th node (when NP is not equal to zero and J equals zero) or the J-th junction (when NP equals zero and J is not equal to zero). The right-hand sides are defined as follows.

For the case at the NP-th node:

(1) For dissolved chemicals:

$$RHSC_i = \left[M_i^{cw} + Ak_i^{ab} p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n A C_{ni}^{s} + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n P C_{ni}^{b} + \sum_{m=1}^{N_{rx}} k_m^{rb} A \prod_{j=1}^{N_c} (C_j^{w})^{b_{mj}} + M_i^{crw} - M_i^{ciw} + M_i^{cow} \right]$$
$$- \left[\lambda_i^{w} A + Ak_i^{af} + \sum_{n=1}^{N_s} S_n A k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n P k_{ni}^{bf} + \sum_{m=1}^{N_{rx}} k_m^{rf} A (C_i^{w})^{a_{mi}-1} \prod_{j=1, j\neq i}^{N_c} (C_j^{w})^{a_{mj}} + R - I + R_1 + R_2 \right] C_i^{w} \qquad \text{(II.52)}$$
$$i \in [1, N_c]$$

(2) For particulate chemicals on suspended sediments:

$$RHSC_k = \left[M_{ni}^{cs} + k_{ni}^{sf} S_n A C_i^{w} + BR_n C_{ni}^{b} - BD_n C_{ni}^{s} + M_{ni}^{cos} \right]$$
$$- \left[\lambda_{ni}^{s} A + k_{ni}^{sb} A + R - I + R_1 + R_2 \right] S_n C_{ni}^{s} \qquad \text{(II.53)}$$
$$n \in [1, N_s],\ i \in [1, N_c],\quad k = n * N_c + i$$

(3) For particulate chemicals on bed sediments:

$$RHSC_k = \left[D_n C_{ni}^{s} - R_n C_{ni}^{b} + k_{ni}^{bf} M_n C_i^{w} \right] - \left[\lambda_{ni}^{b} + k_{ni}^{bb} \right] M_n C_{ni}^{b} \qquad \text{(II.54)}$$
$$n \in [1, N_s], i \in [1, N_c],\quad k = (n + N_s) * N_c + i$$

(4) For suspended sediments:

(a) when ID = 21,

$$RHSS_n = \left[M_n^s + PR_n - PD_n + M_n^{os}\right] - \left[R - I + R_1 + R_2\right]S_n \qquad n \in [1,N_s] \qquad \text{(II.55)}$$

(b) when ID = 22,

$$RHSS_n = \left[M_n^s + PR_n - PD_n + M_n^{os}\right] \qquad n \in [1,N_s] \qquad \text{(II.56)}$$

For the case at the J-th junction:

(1) For dissolved chemicals:

$$RHSC_i =$$

$$\sum_{k=1}^{NJRTH(J)} Q^k C_i^{wk} + M_i^{cw}(J) - \lambda_i^w V(J) C_i^w(J) + M_i^{crw}(J) - M_i^{ciw}(J) + M_i^{cow}(J) + V(J) k_i^{ab}\left[p_i - \frac{k_i^{af}}{k_i^{ab}} C_i^w(J)\right]$$

$$+ \sum_{n=1}^{N_s} k_{ni}^{sb} S_n(J) V(J)\left[C_{ni}^s(J) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w(J)\right] + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n(J) AJT(J)\left[C_{ni}^b(J) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w(J)\right] \qquad \text{(II.57)}$$

$$+ \sum_{m=1}^{N_{rx}} k_m^{rb} V(J)\left[\prod_{j=1}^{N_c} \left(C_j^w(J)\right)^{b_{mj}} - \frac{k_m^{rf}}{k_m^{rb}} \prod_{j=1}^{N_c} \left(C_j^w(J)\right)^{a_{mj}}\right] \qquad i \in [1,N_c]$$

(2) For particulate chemicals on suspended sediments:

$$RHSC_k = \sum_{k=1}^{NJRTH(j)} Q^k S_n C_{ni}^{sk} + M_{ni}^{cs}(J) - \lambda_{ni}^s V(J) S_n(J) C_{ni}^s(J) - k_{ni}^{sb} S_n(J) V(J)\left[C_{ni}^s(J) - \frac{k_{ni}^{sf}}{k_{ni}^{sb}} C_i^w(J)\right] \qquad \text{(II.58)}$$

$$+ R_n(J) AJT(J) C_{ni}^b(J) - D_n(J) AJT(J) C_{ni}^s(J) + M_{ni}^{cos}(J) \qquad n \in [1,N_s],\ i \in [1,N_c],\ k = n * N_c + i$$

(3) For particulate chemicals on bed sediments:

$$RHSC_k = [D_n(J) C_{ni}^s(J) - R_n(J) C_{ni}^b(J)) - \lambda_{ni}^b(J) M_n(J) C_{ni}^b(J) - k_{ni}^{bb} M_n(J)\left[C_{ni}^b(J) - \frac{k_{ni}^{bf}}{k_{ni}^{bb}} C_i^w(J)\right] \qquad \text{(II.59)}$$

$$n \in [1,N_s], i \in [1,N_c], \quad k = (n + N_s) * N_c + i$$

(4) For suspended sediments:

$$RHSS_n = \sum_{k=1}^{NJRTH(j)} Q^k S_n^k + M_n^s(J) + M_n^{os}(J) + [R_n(J) - D_n(J)] AJT(J) \qquad n \in [1,N_s] \qquad \text{(II.60)}$$

Subroutine RHSCMP_2

This subroutine is to compute the right-hand side of the 2-D transport governing equations

of (1) dissolved chemicals (ID = 1), (2) particulate chemicals on suspended sediments (ID = 1), (3) particulate chemicals on bed sediments (ID = 1), and (4) suspended sediments (ID = 21 or 22) at the NP-th node. The right-hand sides are defined as follows.

(1) For dissolved chemicals:

$$RHSC_i = \left[M_i^{cw} + hk_i^{ab}p_i + \sum_{n=1}^{N_s} k_{ni}^{sb} S_n h C_{ni}^{s} + \sum_{n=1}^{N_s} k_{ni}^{bb} M_n C_{ni}^{b} + \sum_{m=1}^{N_{rx}} k_m^{rb} h \prod_{j=1}^{N_c} (C_j^{w})^{b_{mj}} + M_i^{crw} - M_i^{ciw}\right]$$
$$-\left[\lambda_i^{w} h + hk_i^{af} + \sum_{n=1}^{N_s} S_n h k_{ni}^{sf} + \sum_{n=1}^{N_s} M_n k_{ni}^{bf} + \sum_{m=1}^{N_{rx}} k_m^{rf} h (C_i^{w})^{a_{mi}-1} \prod_{j=1, j\neq i}^{N_c} (C_j^{w})^{a_{mj}} + R - I\right] C_i^{w} \quad i \in [1, N_c] \tag{II.61}$$

(2) For particulate chemicals on suspended sediments:

$$RHSC_k = \left[M_{ni}^{cs} + k_{ni}^{sf} h S_n C_i^{w} + R_n C_{ni}^{b} - D_n C_{ni}^{s}\right] - \left[\lambda_{ni}^{s} h + k_{ni}^{sb} h + R - I\right] S_n C_{ni}^{s}$$
$$n \in [1, N_s],\ i \in [1, N_c],\quad k = n * N_c + i \tag{II.62}$$

(3) For particulate chemicals on bed sediments:

$$RHSC_k = \left[D_n C_{ni}^{s} - R_n C_{ni}^{b} + k_{ni}^{bf} M_n C_i^{w}\right] - \left[\lambda_{ni}^{b} + k_{ni}^{bb}\right] M_n C_{ni}^{b}$$
$$n \in [1, N_s], i \in [1, N_c],\quad k = (n + N_s) * N_c + i \tag{II.63}$$

(4) For suspended sediments:

(a) when ID = 21,

$$RHSS_n = \left[M_n^{s} + R_n - D_n\right] - [R - I] S_n \qquad n \in [1, N_s] \tag{II.64}$$

(b) when ID = 22,

$$RHSS_n = \left[M_n^{s} + R_n - D_n\right] \qquad n \in [1, N_s] \tag{II.65}$$

Subroutine RINCS

This subroutine is to read in chemistry and sediment information.

Subroutine RINF_1

This subroutine is to read in information for 1-D river/stream flow simulations.

Subroutine RINF_2

This subroutine is to read in information for 2-D overland flow simulations.

Subroutine RINIT11

This subroutine is to read in the initial condition for the 1-D vertical subsurface flow

simulations that are corresponding to river/stream nodes.

Subroutine RINIT12

This subroutine is to read in the initial condition for the 1-D vertical subsurface flow simulations that are corresponding to overland nodes.

Subroutine RINIT_1

This subroutine is to read in the initial condition for 1-D river/stream flow and/or transport simulations.

Subroutine RINIT_2

This subroutine is to read in the initial condition for 2-D overland flow and/or transport simulations.

Subroutine RINPUT11

This subroutine is to read in information for the 1-D vertical subsurface flow simulations that are corresponding to river/stream nodes.

Subroutine RINPUT12

This subroutine is to read in information for the 1-D vertical subsurface flow simulations that are corresponding to overland nodes.

Subroutine RINT_1

This subroutine is to read in information for 1-D river/stream transport.

Subroutine RINT_2

This subroutine is to read in information for 2-D overland transport.

Subroutine SOL_BS

This subroutine is to solve the transport governing equation of bed sediments at the NP-th river/stream or overland node.

Subroutine SOL_BSJT

This subroutine is to solve the transport governing equation of bed sediments at the IJT-th junction..

Subroutine SOL_C1

This subroutine is to solve for the concentrations of dissolved chemicals, particulate chemicals on suspended sediments, and particulate sediments on bed sediments at 1-D global nodes (ID = 1) or at junctions (ID = 2). For the case at global nodes, this subroutine serves as the corrector step in our predictor-corrector approach to solve transport equations of chemicals. For the case at junctions, the governing equations accounting for chemical interactions are solved in this subroutine. The Newton-Raphson method is employed to solve the nonlinear system of chemical reactions. The full-pivoting technique is incorporated into a direct solver to handle linearized matrix equations.

Subroutine SOL_C2

This subroutine is to solve for the concentrations of dissolved chemicals, particulate chemicals on suspended sediments, and particulate sediments on bed sediments at 2-D global nodes. This subroutine serves as the corrector step in our predictor-corrector approach to solve transport equations of chemicals. The Newton-Raphson method is employed to solve the nonlinear system of chemical reactions. The full-pivoting technique is incorporated into a direct solver to handle linearized matrix equations.

Subroutine SOL_SS1

This subroutine is to solve the transport governing equation of suspended sediments at the NP-th river/stream node, where the time-implicit scheme is employed.

Subroutine SOL_SS2

This subroutine is to solve the transport governing equation of suspended sediments at the NP-th overland node, where the time-implicit scheme is employed.

Subroutine SOL_SSJT

This subroutine is to solve the transport governing equation of suspended sediments at the IJT-th junction, where the time-implicit scheme is employed.

Subroutine SPROP_1

This subroutine is to compute hydraulic conductivity and water capacity in the river/stream node-associated 1-D vertical subsurface simulations.

Subroutine SPROP_2

This subroutine is to compute hydraulic conductivity and water capacity in the overland node-associated 1-D vertical subsurface simulations.

Subroutine STAR2M

This subroutine is to determine the Lagrangian values (i.e., H_1^*, u_1^*, v_1^*, H_2^*, u_2^*, v_2^*, H_3^*, u_3^*, v_3^* appeared in Section 3.2.1) associated with each characteristic.

Subroutine STORE_1

This subroutine is to store the computer results of 1-D river/stream, in relation to the post-processor of Watershed Modeling System (WMS).

Subroutine STORE_2

This subroutine is to store the computer results of 2-D overland, in relation to the post-processor of Watershed Modeling System (WMS).

Subroutine STORE_1D

This subroutine is to store the computer results of 1-D river/stream in a binary file for further plotting purposes.

Subroutine STORE_2D

This subroutine is to store the computer results of 2-D overland in a binary file for further plotting purposes.

Subroutine STRIP

This subroutine is to read in a character variable.

Subroutine SURE_2

This subroutine is to analytically determine the target location of a 2-D tracking path when the single-velocity approach is applied.

Subroutine SURE2M

This subroutine is to analytically determine the target location of a 2-D tracking path when the single-velocity approach is applied. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine SURF_2

This subroutine is to generate boundary arrays for implementing boundary conditions in 2-D simulations.

Subroutine TRAK_V1

This subroutine is to determine the tracking velocity for implementation of the Lagrangian step of 1-D river/stream flow computation

Subroutine TRAK_1

This subroutine is to determine the target location of a tracking path in a 1-D subelement.

Subroutine TRAK_21

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is where an subelement node is located.

Subroutine TRAK_22

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is not where an subelement node is located.

Subroutine TRAK21M

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is where an subelement node is located. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine TRAK22M

This subroutine is to determine (1) whether or not a particle will pass through the working subelement being considered and (2) the location of the target location if the particle will pass through the working subelement. This subroutine is employed when the starting location is not where an subelement node is located. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine TRANSP_1

This subroutine serves as the control panel to compute both contaminant and sediment transport of 1-D river/stream. The predictor-corrector numerical approach is employed to solve the transport equations of mobile materials, such as dissolved chemicals, suspended sediments, and

particulate chemicals on suspended sediments. During each time step, The predictor step is first implemented to obtain the intermediate values for mobile materials. Sediment equations are then solved by using the Picard to handle their nonlinearity. The concentrations of contaminants are the last to solve for. The set of nonlinear algebraic equations is solved with the Newton-Raphson method node by node in the corrector step.

Subroutine TRANSP_2

This subroutine serves as the control panel to compute both contaminant and sediment transport of 2-D overland. The predictor-corrector numerical approach is employed to solve the transport equations of mobile materials, such as dissolved chemicals, suspended sediments, and particulate chemicals on suspended sediments. During each time step, The predictor step is first implemented to obtain the intermediate values for mobile materials. Sediment equations are then solved by using the Picard to handle their nonlinearity. The concentrations of contaminants are the last to solve for. The set of nonlinear algebraic equations is solved with the Newton-Raphson method node by node in the corrector step.

Subroutine TRILRN2M

This subroutine is to generate pointer arrays for the use in constructing the matrix equation for adjusting 2-D flow velocity in the last part of the method of characteristic approach.

Subroutine TSCONV

This subroutine is to retrieve desired profiles from given x-y series curves.

Subroutine TSCONVV

This subroutine is to retrieve desired profiles from given x-y series curves.

Subroutine TSCONV2

This subroutine is to retrieve desired profiles from given x-y series curves.

Subroutine VALBDL_2

This subroutine is to compute the velocity at a specified 2-D node by interpolation.

Subroutine VALBDL2M

This subroutine is to compute the velocity at a specified 2-D node by interpolation. It is used only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine VELTGW1

This subroutine is to calculate the velocity at all nodes in the river/stream node-associated 1-D vertical subsurface simulations.

Subroutine VELTGW2

This subroutine is to calculate the velocity at all nodes in the overland node-associated 1-D vertical subsurface simulations.

Subroutine VELT_1

This subroutine is to compute the kinematic or diffusion velocities at all river/stream nodes.

Subroutine VELT_2

This subroutine is to compute the kinematic or diffusion velocities at all overland nodes.

Subroutine WRKARY_2

This subroutine is to prepare working arrays for particle tracking in either a 2-D element or a 2-D subelement.

Subroutine WRKARY2M

This subroutine is to prepare working arrays for particle tracking in either a 2-D element or a 2-D subelement. It is employed only when the method of characteristics is employed to solve the 2-D flow equation.

Subroutine XSI_2

This subroutine is to determine the local coordinates of a specified node that is located in a 2-D element, given the original Cartesian coordinates of both the node and element nodes.

APPENDIX C PARAMETERS FOR RUNNING THE COMPUTER CODE

The following is the content of the including file, **wmpara12.inc**, which is required to compile and run the computer code of the model. One needs to modify wmpara12.inc in order to provide appropriate values for the code parameters as defined as follows.

```
C
C ----- CONTROL INTEGERS FOR THE SPATIAL DOMAIN OF 2-D OVERLAND FLOW
C
C  MAXNPK2  : MAX. NO. OF NODES
C  MAXELK2  : MAX. NO. OF ELEMENTS
C  MXBNPK2  : MAX. NO. OF BOUNDARY NODAL POINTS
C  MXBESK2  : MAX. NO. OF BOUNDARY-ELEMENT SURFACES
C    MXJBDK2   : MAX. NO. OF NONZERO ELEMENTS IN ANY ROW FOR NODE-WISE
CONNECTIVITY
C    MXKBDK2   : MAX. NO. OF NONZERO ELEMENTS IN ANY ROW FOR ELEMENT-WISE
CONNECTIVITY
C
     PARAMETER (MAXNPK2=275,MAXELK2=462,MXBNPK2=1000,MXBESK2=1000)
     PARAMETER (MXJBDK2=20,MXKBDK2=20)
C
C ----- CONTROL INTEGERS FOR THE TIME DOMAIN OF 2-D OVERLAND FLOW
C
C  MXNTIK2  : MAX. NO. OF TIME STEPS
C  MXDTCK2  : MAX. NO. OF CHANGES OF THE 2-D TIME STEP SIZE.
C
     PARAMETER (MXNTIK2=50000,MXDTCK2=20)
C
C ----- CONTROL INTEGERS FOR MATERIAL PROPERTIES OF 2-D OVERLAND FLOW
C
C  MXMATK2  : MAX. NO. OF MATERIAL TYPES
C  MXMPMK2  : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL
C
     PARAMETER (MXMATK2=10,MXMPMK2=6)
C
C ----- CONTROL INTEGERS FOR RAINFALL OF 2-D OVERLAND FLOW
C
C  MXRESK2  : MAX. NO. OF ELEMENTS WITH RAINFALL CONDITION
C  MXRPRK2  : MAX. NO. OF RAINFALL PROFILES
C  MXRDPK2  : MAX. NO. OF DATA POINTS ON THE RAINFALL PROFILE
C
     PARAMETER (MXRESK2=MAXELK2,MXRPRK2=5,MXRDPK2=200)
C
C ----- CONTROL INTEGERS FOR SOURCE/SINK OF 2-D OVERLAND FLOW
C
C  MXSPRK2  : MAX. NO. OF SOURCE/SINK PROFILES
C  MXSDPK2  : MAX. NO. OF DATA POINTS ON THE SOURCE/SINK PROFILE
C
     PARAMETER (MXSPRK2=5,MXSDPK2=200)
```

```
C
C ----- CONTROL INTEGERS FOR OPEN BOUNDARY CONDITIONS OF 2-D OVERLAND FLOW
C
C  MXDNPK2  : MAX. NO. OF DIRICHLET BOUNDARY NODAL POINTS
C  MXDPRK2  : MAX. NO. OF DIRICHLET BOUNDARY PROFILES
C  MXDDPK2  : MAX. NO. OF DATA POINTS IN A DIRICHLET PROFILES
C  MXCESK2  : MAX. NO. OF FLUX-TYPE BOUNDARY SIDES.
C  MXFPRK2  : MAX. NO. OF UPSTREAM BOUNDARY FLUX PROFILES
C  MXFDPK2  : MAX. NO. OF DATA POINTS IN A UPSTREAM BOUNDARY PROFILE
C  MXCPRK2  : MAX. NO. OF DEPTH- OR STAGE-DEPENDENT FLUX PROFILES
C   MXCDPK2   : MAX. NO. OF DATA POINTS IN A DEPTH- OR STAGE-DEPENDENT FLUX
PROFILE
C
    PARAMETER (MXDNPK2=500,MXDPRK2=10,MXDDPK2=500)
    PARAMETER (MXCESK2=500,MXFPRK2=10,MXFDPK2=300)
    PARAMETER (MXCPRK2=3,MXCDPK2=300)
C
C ----- CONTROL INTEGERS FOR CLOSED BOUNDARY CONDITIONS OF 2-D OVERLAND FLOW
C
C  MXIBPK2  : MAX. NO. OF CLOSED BOUNDARY NODAL POINTS
C
    PARAMETER (MXIBPK2=500)
C
C ----- CONTROL INTEGERS FOR SUB-ELEMENT TRACKING OF 2-D OVERLAND FLOW
C
C  MXNPWK2  : MAX. NO. OF NODES FOR A SUB-ELEMENT TRACKING
C  MXELWK2  : MAX. NO. OF SUB-ELEMENTS FOR A SUB-ELEMENT TRACKING
C
    PARAMETER (MXNPWK2=121,MXELWK2=100)
C
C ----- CONTROL INTEGERS FOR THE SPATIAL DOMAIN OF 1-D SUBSURFACE FLOW
C      CORRESPONDING TO 2-D OVERLAND NODES
C
C  MXELGK2  : MAX. NO. OF SUBSURFACE ELEMENTS IN EACH VERTICAL COLUMN
C  MXNPGK2  : MAX. NO. OF NODAL POINTS IN EACH VERTICAL COLUMN
C
    PARAMETER (MXELGK2=40,MXNPGK2=MXELGK2+1)
C
C ----- CONTROL INTEGERS FOR MATERIAL AND SOIL PROPERTIES OF SUBSURFACE FLOW
C      CORRESPONDING TO 2-D OVERLAND NODES
C
C  MXMTGK2  : MAX. NO. OF SOIL MATERIAL TYPES
C  MXSPGK2  : MAX. NO. OF SOIL PARAMETERS TO DESCRIBE WATER RETENTION CURVES
C  MXMPGK2  : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL
C  MXNO1K2  : MAX. NO. OF ELEMENTS WITH MATERIAL TYPE OTHER THAN 1
C
    PARAMETER (MXMTGK2=10,MXSPGK2=25,MXMPGK2=6,MXNO1K2=100)
C
```

```
C ----- CONTROL INTEGERS FOR BOUNDARY CONDITIONS OF SUBSURFACE FLOW
CORRESPONDING
C     TO 2-D OVERLAND NODES
C
C  MXPRFK2  : MAX. NO. OF BOUNDARY PROFILES
C  MXBDPK2  : MAX. NO. OF DATA POINTS ON THE PROFILE
C
     PARAMETER (MXPRFK2=2,MXBDPK2=4)
C
C ----- CONTROL INTEGERS FOR HYDROGRAPH OF 2-D OVERLAND FLOW
C
C  MXPNTK2  : MAX. NO. OF NODAL POINTS FOR THE LINE CROSS SECTION
C  MXLINK2  : MAX. NO. OF LINE CROSS SECTION CAN BE SELECTED
C  MXITPK2  : MAX. NO. OF DATA POINTS ON THE HYDROGRAPH
C
     PARAMETER (MXPNTK2=50,MXLINK2=10,MXITPK2=100)
C
C ----- CONTROL INTEGERS FOR 2-D OVERLAND TRANSPORT
C
C  MXMMMK2  : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL FOR TRANSPORT
C  MXSRPRK2 : MAX. NO. OF SOURCE/SINK PROFILES
C  MXSRDPK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A SOURCE/SINK PROFILE
C  MXCESTK2 : MAX. NO. OF FLUX-TYPE BOUNDARY SIDES OF TRANSPORT
C  MXCPRTK2 : MAX. NO. OF FLUX-TYPE BOUNDARY CONDITION PROFILES OF TRANSPORT
C  MXCDPTK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A FLUX-TYPE BOUNDARY
C          CONDITION PROFILE OF TRANSPORT
C  MXDNPTK2 : MAX. NO. OF DIRICHLET BOUNDARY NODES OF TRANSPORT
C  MXDPRTK2 : MAX. NO. OF DIRICHLET BOUNDARY CONDITION PROFILES OF TRANSPORT
C  MXDDPTK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A DIRICHLET BOUNDARY
C          CONDITION PROFILE OF TRANSPORT
C  MXRCPRK2 : MAX. NO. OF CHEMICAL CONCENTRATION PROFILES IN RAINFALL
C     MXRCDPK2 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A CHEMICAL
CONCENTRATION
C          PROFILES IN RAINFALL
C
     PARAMETER (MXMMMK2=3)
     PARAMETER (MXSRPRK2=20,MXSRDPK2=20)
     PARAMETER (MXRCPRK2=20,MXRCDPK2=20)
     PARAMETER (MXDNPTK2=200,MXDPRTK2=200,MXDDPTK2=100)
     PARAMETER (MXCESTK2=200,MXCPRTK2=200,MXCDPTK2=100)
C
C ----- CONTROL INTEGERS FOR THE SPATIAL DOMAIN OF 1-D RIVER/STREAM FLOW
C
C  MAXNPK1  : MAX. NO. OF NODES
C  MAXELK1  : MAX. NO. OF ELEMENTS
C
     PARAMETER (MAXNPK1=500,MAXELK1=500)
C
```

```
C ----- CONTROL INTEGERS FOR THE TIME DOMAIN OF 1-D RIVER/STREAM FLOW
C
C  MXNTIK1  : MAX. NO. OF TIME STEPS
C  MXDTCK1  : MAX. NO. OF CHANGES OF THE 1-D TIME STEP SIZE
C
     PARAMETER (MXNTIK1=5000,MXDTCK1=20)
C
C ----- CONTROL INTEGERS FOR MATERIAL PROPERTIES OF 1-D RIVER/STREAM FLOW
C
C  MXMATK   : MAX. NO. OF MATERIAL TYPES
C  MXMPMK   : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL
C
     PARAMETER (MXMATK1=10,MXMPMK1=6)
C
C ----- CONTROL INTEGERS FOR RAINFALL OF 1-D RIVER/STREAM FLOW
C
C  MXRESK1  : MAX. NO. OF ELEMENTS WITH RAINFALL CONDITION
C  MXRPRK1  : MAX. NO. OF RAINFALL PROFILES
C  MXRDPK1  : MAX. NO. OF DATA POINTS ON THE RAINFALL PROFILE
C
     PARAMETER (MXRESK1=MAXELK1,MXRPRK1=5,MXRDPK1=200)
C
C ----- CONTROL INTEGERS FOR SOURCE/SINK OF 1-D RIVER/STREAM FLOW
C
C  MXSPRK1  : MAX. NO. OF SOURCE/SINK PROFILES
C  MXSDPK1  : MAX. NO. OF DATA POINTS ON THE SOURCE/SINK PROFILE
C  MXSJPRK1 : MAX. NO. OF SOURCE/SINK PROFILES AT JUNCTIONS
C  MXSJDPK1 : MAX. NO. OF DATA POINTS ON THE SOURCE/SINK PROFILE AT JUNCTIONS
C
     PARAMETER (MXSPRK1=5,MXSDPK1=200)
     PARAMETER (MXSJPRK1=5,MXSJDPK1=200)
C
C ---- CONTROL INTEGERS FOR OPEN BOUNDARY CONDITIONS OF 1-D RIVER/STREAM FLOW
C
C  MXDNPK1  : MAX. NO. OF OPEN BOUNDARY NODAL POINTS
C  MXDPRK1  : MAX. NO. OF OPEN BOUNDARY PROFILES
C  MXDDPK1  : MAX. NO. OF DATA POINTS ON THE PROFILES
C
     PARAMETER (MXDNPK1=500,MXDPRK1=50,MXDDPK1=300)
     PARAMETER (MXCPRK1=10,MXCDPK1=300)
C
C ----- CONTROL INTEGERS FOR 1-D RIVER/STREAM REACH NUMBER
C
C  MXRHK1   : MAX. NO. OF RIVER/STREAM REACH NUMBER
C  MXRHNPK1 : MAX. NO. OF NODES INCLUDED IN A RIVER/STREAM REACH
C
     PARAMETER (MXRHK1=10,MXRHNPK1=100)
C
```

```
C ----- CONTROL INTEGERS FOR CROSS-SECTIONAL GEOMETRY FOR 1-D RIVER/STREAM
FLOW
C
C  MXCNPK1  : MAX. NO. OF DATA POINTS FOR CROSS-SECTIONAL GEOMETRY PROFILES
C
     PARAMETER (MXCNPK1=200)
C
C ----- CONTROL INTEGERS FOR RIVER/STREAM JUNCTIONS
C
C  MXJTK1   : MAX. NO. OF RIVER/STREAM JUNCTIONS
C  MXJTRK1  : MAX. NO. OF RIVER/STREAM REACHES CONNECTED TO A JUNCTION
C  MXJTPK1  : MAX. NO. OF RIVER/STREAM JUNCTION PROFILES
C  MXJTDK1  : MAX. NO. OF DATA POINTS ON THE PROFILES
C  MXNJTSK1 : MAX. NO. OF JUNCTION-RELATED OVERLAND BOUNDARY SIDES
C          TO A JUNCTION.
C
     PARAMETER (MXJTK1=500,MXJTRK1=50,MXJTPK1=50,MXJTDK1=100)
     PARAMETER (MXNJTSK1=50)
C
C ----- CONTROL INTEGERS FOR SUB-ELEMENT TRACKING FOR 1-D RIVER/STREAM FLOW
C
C  MXNPWK1  : MAX. NO. OF NODES FOR A SUB-ELEMENT TRACKING
C
     PARAMETER (MXNPWK1=11)
C
C ----- CONTROL INTEGERS FOR THE SPATIAL DOMAIN OF 1-D SUBSURFACE FLOW
C      CORRESPONDING TO 1-D RIVER/STREAM NODES
C
C  MXELGK1  : MAX. NO. OF SUBSURFACE ELEMENTS IN EACH VERTICAL COLUMN
C  MXNPGK1  : MAX. NO. OF NODAL POINTS IN EACH VERTICAL COLUMN
C
     PARAMETER (MXELGK1=40,MXNPGK1=MXELGK1+1)
C
C ----- CONTROL INTEGERS FOR MATERIAL AND SOIL PROPERTIES OF SUBSURFACE FLOW
C      CORRESPONDING TO 1-D RIVER/STREAM NODES
C
C  MXMTGK1  : MAX. NO. OF SOIL MATERIAL TYPES
C  MXSPGK1  : MAX. NO. OF SOIL PARAMETERS TO DESCRIBE WATER RETENTION CURVE
C  MXMPGK1  : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL
C  MXNO1K1  : MAX. NO. OF ELEMENTS WITH MATERIAL TYPE OTHER THAN 1
C
     PARAMETER (MXMTGK1=10,MXSPGK1=25,MXMPGK1=6,MXNO1K1=100)
C
C ----- CONTROL INTEGERS FOR BOUNDARY CONDITIONS OF SUBSURFACE FLOW
CORRESPONDING
C      TO 1-D RIVER/STREAM NODES
C
C  MXPRFK1  : MAX. NO. OF BOUNDARY PROFILES
```

```
C  MXBDPK1  : MAX. NO. OF DATA POINTS ON THE PROFILE
C
      PARAMETER (MXPRFK1=2,MXBDPK1=4)
C
C ----- CONTROL INTEGERS FOR HYDROGRAPH OF 1-D RIVER/STREAM FLOW
C
C  MXPNTK1  : MAX. NO. OF NODAL POINTS FOR THE LINE CROSS SECTION
C  MXLINK1  : MAX. NO. OF LINE CROSS SECTION CAN BE SELECTED
C  MXITPK1  : MAX. NO. OF DATA POINTS ON THE HYDROGRAPH
C
      PARAMETER (MXPNTK1=50,MXLINK1=10,MXITPK1=100)
C
C ----- CONTROL INTEGERS FOR 1-D RIVER/STREAM TRANSPORT
C
C  MXMMMK1  : MAX. NO. OF MATERIAL PROPERTIES PER MATERIAL FOR TRANSPORT
C  MXSRPRK1 : MAX. NO. OF SOURCE/SINK PROFILES
C  MXSRDPK1 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A SOURCE/SINK PROFILE
C  MXSJRTK1 : MAX. NO. OF SOURCE/SINK PROFILES OF TRANSPORT AT JUNCTIONS
C  MXSJDTK1 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A SOURCE/SINK PROFILE
C          OF TRANSPORT AT JUNCTIONS.
C  MXDNPTK1 : MAX. NO. OF DIRICHLET BOUNDARY NODES OF TRANSPORT
C  MXBPPRK1 : MAX. NO. OF BOUNDARY CONDITION PROFILES
C  MXBPDPK1 : MAX. NO. OF DATA POINTS USED TO DESCRIBE A BOUNDARY CONDITION
PROFILE
C  MXRCPRK1 : MAX. NO. OF CHEMICAL CONCENTRATION PROFILES IN RAINFALL.
C     MXRCDPK1  : MAX. NO. OF DATA POINTS USED TO DESCRIBE A CHEMICAL
CONCENTRATION
C          PROFILES IN RAINFALL
C
      PARAMETER (MXMMMK1=2)
      PARAMETER (MXSRPRK1=20,MXSRDPK1=20)
      PARAMETER (MXSJRTK1=5,MXSJDTK1=200)
      PARAMETER (MXBPPRK1=20,MXBPDPK1=20)
      PARAMETER (MXAPPRK1=20,MXAPDPK1=20)
      PARAMETER (MXRCPRK1=20,MXRCDPK1=20)
      PARAMETER (MXDNPTK1=20)
C
C ----- CONTROL INTEGERS FOR CHEMICAL AND SEDIMENT TRANSPORT
C
C  MXNRXK   : MAX. NO. OF CHEMICAL REACTIONS
C  MXNCHK   : MAX. NO. OF DISSOLVED CHEMICALS
C  MXNSIK   : MAX. NO. OF SEDIMENT SIZES
C  MXTNCK   : MAX. NO. OF DISSOLVED AND PARTICULATE CHEMICALS
C  MXTNSK   : MAX. NO. OF SUSPENDED AND BED SEDIMENT SIZES
C  MXTSRK    : MAX. NO. OF DISSOLVED CHEMICALS, SUSPENDED SEDIMENTS, AND
PARTICULATE
C          CHEMICALS ON THE SUSPENDED SEDIMENT
C  MXAPPRK  : MAX. NO. OF PARTIAL ATMOSPHERIC PRESSURE PROFILES
```

```
C  MXAPDPK  : MAX. NO. OF DATA POINTS USED TO DESCRIBE A PARTIAL ATMOSPHERIC
C            PRESSURE
C
      PARAMETER (MXNRXK=10,MXNCHK=10,MXNSIK=5)
      PARAMETER (MXTNCK=MXNCHK*(MXNSIK*2+1),MXTNSK=MXNSIK*2)
      PARAMETER (MXTSRK=MXNCHK+MXNSIK+MXNCHK*MXNSIK)
      PARAMETER (MXAPPRK=20,MXAPDPK=20)
C
C ----- CONTROL INTEGERS FOR DESCRIBING FUNCTIONAL CURVES
C
C  MXXYSK   : MAX. NO. OF CURES/SERIES
C  MXXYPK   : MAX. NO. OF DATA POINTS FOR THE CURVES
C
      PARAMETER (MXXYSK=300,MXXYPK=500)
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13. ABSTRACT ***(Maximum 200 words)***

This report presents the development of a numerical model simulating water flow, contaminant transport, and sediment transport in watershed systems. The model is composed of two modules: flow and transport. Three options are provided in modeling the flow module in river/stream network and overland regime: the kinematic wave approach, diffusion wave approach, and dynamic wave approach. The kinematic and diffusion wave approaches are known to be numerically robust in terms of numerical convergency and stability, i.e., they can generate convergent and stable simulations over a wide range of ground surface slopes in the entire watershed. The question is the accuracy of these simulations. The kinematic wave approach usually produces accurate solutions only over the region of steep slopes. The diffusion wave approach normally gives accurate solutions over the region of mild to steep slopes. However, neither approach has the ability to yield accurate solutions over the region of small slopes, in which the inertial forces are no longer negligible compared with the gravitational forces. The kinematic wave approach cannot even address the problems of backwater effects. On the other hand, a dynamic wave approach, having included all forces, can theoretically have the potential to generate accurate simulations over all ranges of slopes in a watershed.
(Continued)

14. SUBJECT TERMS

Contaminant and sediment transport
Darcy's velocity
Diffusion wave
Galerkin finite element method
Interaction between overland and subsurface flow
Manning's equation
One-dimensional river/stream network
Overland flow
Richard's equation
Subsurface flow
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A total of eight groups of example problems were given in this report to demonstrate the capability of this model. Continuing work is underway to incorporate a three-dimensional subsurface flow and chemical transport model into this watershed model. The Richards' equation and advection-dispersion reactive chemical transport equations will form the basis to simulate the subsurface flow and chemical transport module in saturated-unsaturated media. The computational module of subsurface flow and reactive chemical transport will be developed based on a model of coupled density dependent flow and chemical transport through saturated-unsaturated media.