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MASS2
Modular Aquatic Simulation System in Two Dimensions

User Guide and Reference

W. A. Perkins
M. C. Richmond

September 2004

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RL01830

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Preface

This manual documents the use of the Modular Aquatic Simulation System in Two Dimensions (MASS2). It is the second of two reports on MASS2. The first report documents the theory and numerical methods used in MASS2, and is often referred to herein as the Theory Manual.

This manual contains many examples of computer files and their content. Any fixed file name or what may be contained in computer files is highlighted using `fixed width` type. A **`bold fixed width`** type is used to highlight what the user might enter during an interactive session.

This document was prepared so that it can be easily viewed on a computer using the Adobe Portable Document Format (PDF). All cross references, citations, and Internet addresses are "hot" links. Clicking on them will cause your document viewer to take you directly to that destination, whether it be in this document, the Theory Manual, or on the Internet.

Acknowledgments

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1.0 Introduction

The Modular Aquatic Simulation System in Two Dimensions (MASS2) is a two-dimensional, depth-averaged hydrodynamics and transport model that simulates time varying distributions of depth-averaged velocities, water surface elevations, and water quality constituents. MASS2 is applicable to a wide variety of environmental analyses of rivers and estuaries where vertical variations in the water column are negligible or unimportant. For example, MASS2 has been applied to simulate the water quality effects of altered total dissolved gas production at Columbia and Snake River dams (Richmond et al. 1999, 2000); juvenile chinook salmon habitat, and its variation in time, along the Hanford Reach of the Columbia River (McMichael et al. 2003; Perkins et al. 2004, and); and the fate of Hanford Site radionuclides should they enter the Columbia River (Kincaid et al. 2001).

MASS2 is formulated using the general finite-volume principles described by Patankar (1980). The model uses a structured multi-block scheme employing a curvilinear computational mesh. The coupling of the momentum and mass conservation (continuity) equations is achieved using a variation of the SIMPLE algorithm (Patankar 1980) extended to shallow-water flows by Zhou (1995). Spasojevic and Holly (1990) give another example of a two-dimensional model of this type.

This document is the second of a set of two describing MASS2. The first (Perkins and Richmond 2004) describes the underlying theory and numerical methods used in MASS2 and is referred to here as the "Theory Manual." Before using MASS2, the reader should have a basic understanding of the physical theory described in the Theory Manual. A complete description of the theory and numerical methods used in MASS2 is presented in the companion Theory Manual (Perkins and Richmond 2004). The reader should also understand that this document does not attempt to convey the experience and judgment required for the meaningful application of MASS2 or other similar hydrodynamic and transport model.

This manual is divided into three parts. The first part (Chapter 2) is a general description of the model, its features, and its general use. The second part (Chapter 3) provides the user with a general procedure for configuring MASS2 to simulate a problem. The third part (Chapters 4 through 6) provide detailed references for MASS2 input files, output, utility programs. The appendices present working input files from some test (Appendix A) and real world (Appendix B) applications.

The user completely unfamiliar with MASS2 will want to read Chapter 2 first to get a general feel for the capabilities of the model and the data necessary to use it. Once familiar with the general use of MASS2, the user should then attempt to apply it to a simple problem following the guidelines of Chapter 3 and referring as necessary to the reference chapters. Experienced MASS2 users will use this document for reference.

2.0 Overview of Model Use

This chapter provides a general description of the capabilities of the Modular Aquatic Simulation System in Two Dimensions (MASS2).

2.1 Model Features

MASS2 uses a boundary-fitted, orthogonal, curvilinear computational mesh. One of the features that distinguishes MASS2 from similar models is the ability to use multiple computational mesh blocks. Multiple blocks allow MASS2 to be applied to complex domains. Blocks can be connected to each other with cells having a one-to-one or one-to-many correspondence. This allows the user to use a high-density mesh where detailed results are needed and coarser meshes elsewhere.

MASS2 is designed to simulate a range of river and estuarine flow and water quality problems where vertical velocity and gradients are not important. MASS2 can simulate a wide variety of hydrodynamic conditions, including supercritical flow and hydraulic jumps. MASS2 can also be used to simulate the fate and transport of water quality parameters. Any number of conservative or decaying scalar quantities (e.g., salinity, radionuclides) may be simulated simultaneously with hydrodynamics or precomputed hydrodynamics. In addition, MASS2 has the ability to simulate some special water quality parameters: total dissolved gas, temperature, and suspended sediment.

The model is coded in standard Fortran 90. The code was developed on Silicon Graphics UNIX workstations and under Linux on Intel PCs. It has been used successfully on variety of other platforms as well, like Windows and MacOS X.

2.2 Modes of Operation

MASS2 has several modes of operation so it can adapt to many situations. In the *no simulation* mode, MASS2 reads all necessary input and prepares all specified output, but does not actually perform a simulation. This mode is useful, particularly with the initial configuration of a MASS2 simulation, in identifying and correcting problems with the input. *Hydrodynamics* mode is used to simulate only hydrodynamics, producing estimates of velocity, depth, and water surface elevation. All water quality capabilities are disabled. This mode is used when water quality simulation is not necessary or to prepare hydrodynamic conditions for *transport only* mode. In *transport* mode, the fate and transport of water quality quantities are simulated simultaneously with the hydrodynamics. *Transport-only* mode is used to reduce the run times of water quality simulations by separating the hydrodynamics and transport calculations. This mode is very useful for applications in which water quality is to be simulated over long periods or hydrodynamic conditions vary less over time than water quality or when several water quality situations are to be simulated with the same hydrodynamics. *Transport* mode simulation speed is limited by hydrodynamics, which must run

at a relatively small time step (usually less than 1 minute). Scalar transport, on the other hand, can usually be simulated at a much larger time step (usually 1 or more hours).

2.3 Input Files

MASS2 input consists of several plain text files. The number and names of these files vary depending on the simulation mode and the degree of detail required to describe the application. Figure 2.1 shows required and optional input files used by MASS2 depending on simulation mode. Refer to Chapter 4 for input file format details.

At a minimum, the configuration file, `mass2.cfg`, the hydrodynamics boundary conditions file, `bcspecs.dat`, and files defining the computational mesh are required for all simulation modes. The files `mass2.cfg` and `bcspecs.dat` must exist in the current directory. In hydrodynamics mode, it is usually necessary to define boundary conditions in `bcspecs.dat` that refer to time series files. Additional input files will be used if gage output is specified or spatially varying parameters (like roughness) are necessary.

Transport mode requires `scalar_source.dat` and `scalar_bcspecs.dat` in addition to all of the files used in hydrodynamic mode. The `scalar_source.dat` file defines the transported scalar quantities to be simulated. The `scalar_bcspecs.dat` file defines boundary conditions for transported scalar quantities, usually referring to time series data files. When specific scalar properties require, files may be necessary to define scalar non-point sources, for example. An additional file is required for transport-only mode: `transport_only.dat`. This file contains a list of hot-start files containing hydrodynamic conditions and the simulation time at which they apply. Files with fixed names (`mass2.cfg`, `bcspecs.dat`, etc). are expected to be in the current directory. Other files may reside elsewhere, provided they are specified with a complete, correct path name (which may be relative to the current directory).

2.4 Running MASS2

MASS2 is a command-line program. It does not have any graphical user interface (GUI), although this is under consideration for future versions. The model is usually compiled into an executable named `mass2` (Unix) or `mass2.exe` (Windows). As a command line program, MASS2 execution can be automated with shell scripts or batch files. If used interactively, MASS2 must be run from a shell prompt (Unix, etc.) or a command prompt (Windows). MASS2 produces the following when the simulation is successfully completed:

```
> mass2
 calling mass2_main
 Pacific Northwest National Laboratory

 mass2 code version 0.27

 release: Date: 2004/03/25 22:39:26
```

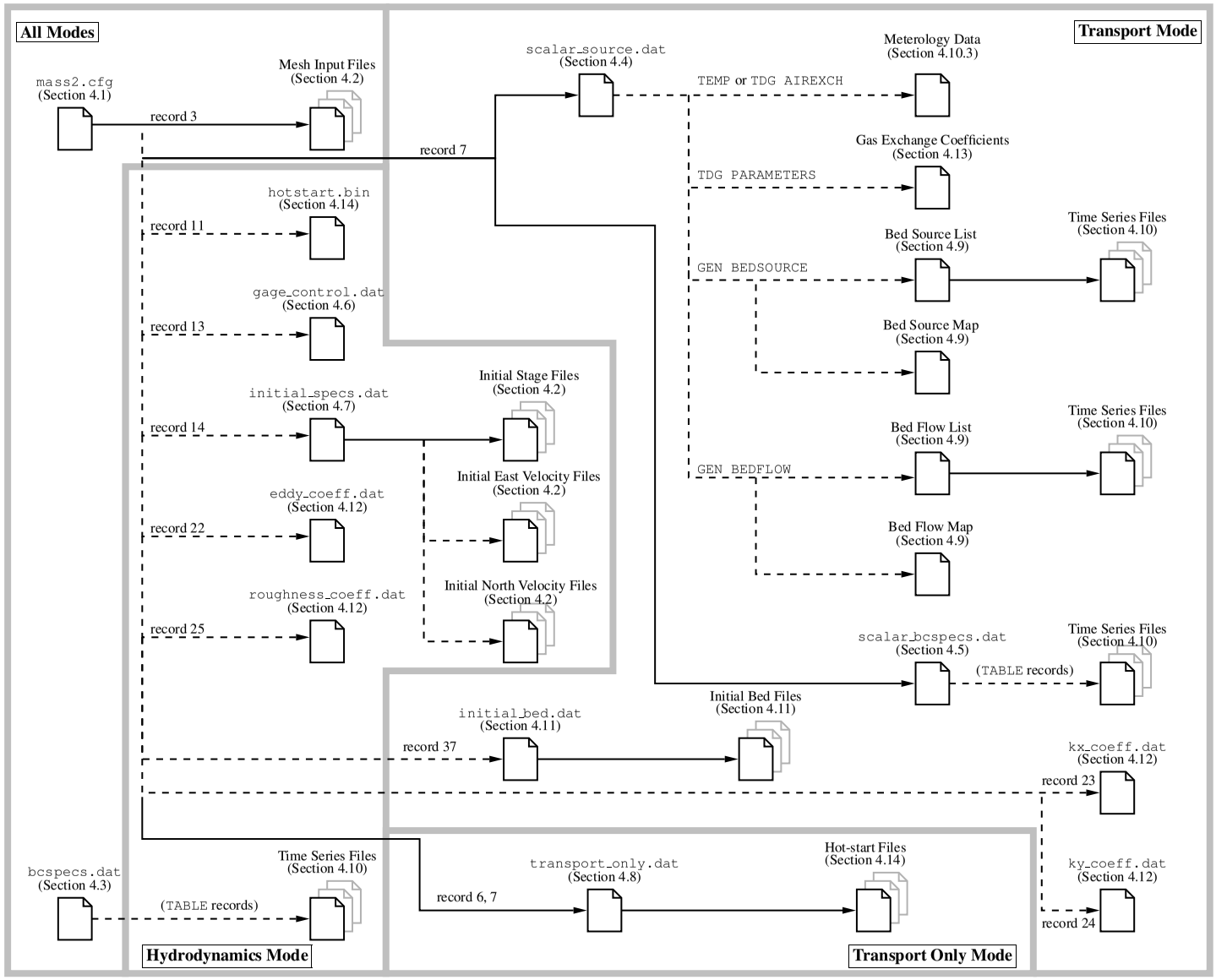


Figure 2.1. Required and optional MASS2 input files. Solid lines indicate files required for the specified mode; dashed lines indicate optional files. Filenames that cannot be set by the user are shown in `fixed width type`.

```
 completion with status=          99
>
```

Serious errors and warnings will also be reported to the screen should they occur. MASS2 has somewhat limited error handling and reporting. Problems arising from input errors or simulations that crash are sometimes difficult to diagnose. This error detection and reporting has improved over time and is an ongoing effort.

2.5 Hydrodynamic Convergence

MASS2 solves for hydrodynamic conditions in an iterative manner (see the Theory Manual, Section 3.3.1). The technique repeatedly solves the momentum and depth correction equations until together they converge to a reasonable solution. The measure used to determine convergence is the "mass source error,"[(a)] which represents the maximum fluid imbalance in the domain. MASS2 reports this imbalance for each block in the domain (Section 5.3). The hydrodynamic solution is considered converged if the mass imbalance of *all* blocks in the domain is less than the user-specified maximum.

Hydrodynamic convergence is controlled by several simulation parameters (Table 2.1) that are used to adjust the rate of convergence. If the rate of convergence is too slow, convergence is never reached. If too fast, the solution can be come unstable. When MASS2 is run "gently," the simulated conditions at the end of one hydrodynamic iteration are very close to the conditions from the previous iteration. This keeps the simulation from becoming unstable. The simulation also requires much longer to converge to the appropriate solution. Aggressive parameters cause simulated conditions to change more rapidly during a hydrodynamic iteration. This can either lead to more rapid convergence or to instability.

Table 2.1. Simulation parameters for gentle and aggressive hydrodynamic solution. The values shown are general approximations. Actual ranges will depend on the specific problem.

Simulation Parameter	Gentle	Aggressive
Time step	small ($\approx$1 sec)	large ($>$ 1 min)
Eddy viscosity	large ($\approx$100 ft^2/sec)	small ($\approx$0.01 ft^2/sec)
Hydrodynamic (outer) iterations	few (3)	more (10)
Depth correction TDMA (inner) iterations	few (15)	more (50)
Depth correction under-relaxation	small (1 – 5%)	large (40%)
Maximum mass source error	large	small (3%)

2.6 Simulation Results

MASS2 can save the current state of the entire simulated domain at regular intervals. The initial and final state of the simulation are always saved. This two-dimensional output is useful

(a) This term was coined by Patankar (1980).

for animations and statistical summaries (e.g., by area) and can be used directly by Tecplot[(b)] to produce high-quality visualizations and animations of the results. A prodigious amount of simulation data can be produced this way. To provide an efficient way to store and handle these data, MASS2 can save it in two file formats specialized to store time series of spatial data: the Network Common Data Form (NetCDF) (Rew et al. 1997) and the Computational Fluid Dynamics (CFD) General Notation System (CGNS) (Rumsey et al. 2002; CGNS Project Group 2003) as described in Section 5.4.

MASS2 can also save the state of a set of individual cells at regular intervals (time series) that may be different than the interval for two-dimensional output. This is called gage output and is used for comparing simulation results to measurements taken by a gage at a known location. Gage output is written to a NetCDF file (Section 5.5) from which data can be extracted using the `mass2gage.pl` script (Section 6.2.1).

The simulation state can be saved in a "hot-start" file (Section 5.6), which is a more complete description of the numerical solution than the two-dimensional output. These hot-start files can be used to initialize a new simulation or in transport-only mode. They can be saved at regular intervals so that if the simulation, or the computer system, crashes, the entire simulation will not be lost.

(b) A commercial scientific visualization package available from Tecplot, Inc.

3.0 Application Setup Guidelines

This chapter supplies the user with a general set of guidelines for configuring and running a complete application for MASS2. Because each application is somewhat different, this chapter lays out some general practices that experience has shown to work. Rather than walking the reader through an oversimplified tutorial, a general process is presented that can be applied to simple and complicated problems alike. The application is presented here in a series of distinct steps:

1. Build a computational grid (Section 3.1).
2. Incrementally create and verify input files with the initial setup (Section 3.2). The initial setup is used to to verify the computational grid, test an initial configuration file and determine boundary and initial conditions, but not perform any simulation.
3. Perform a cold start simulation (Section 3.3). This is the first attempt to simulate hydrodynamics and transition the model from the initial conditions to a more physically reasonable state (usually a steady-state condition).
4. Perform a warmup simulation (Section 3.4). This is used to transition the model from the cold start into unsteady conditions.
5. Perform the desired simulation (Section 3.5).

The beginning user will want to read this entire chapter before attempting a simulation, then use the guidelines in this chapter to assemble and solve a simple, easily verifiable problem. Several data sets are available to use as a guide (Appendix A). A basic understanding of the hydrodynamic solution (Section 3.3.1 of the Theory Manual) is necessary, particularly what constitutes a hydrodynamic iteration and how under-relaxation of the depth correction affects solution. The beginning MASS2 user is advised to use this chapter as follows:

- Read Sections 3.1 through 3.5 to become familiar with the application process.
- Read Section 3.3.1 of the Theory Manual to gain a basic understanding of the hydrodynamic solution, particularly what constitutes an (outer) iteration and how under-relaxation of the depth correction affects solution.
- Choose a simple, easily verifiable hydrodynamics problem to solve with only one computational mesh block, like uniform flow in a rectangular channel (see Section 4.1.1 of the Theory Manual).
- Follow the guidelines in this chapter to set up and simulate the simple problem.
- Upon successful completion of the simple problem, a more realistic problem can be attempted.

3.1 Computational Mesh

The domain simulated by MASS2 is discretized using a boundary-fitted, orthogonal (or nearly orthogonal), curvilinear computational mesh (Theory Manual, Section 2.1). The domain may consist of multiple blocks. Each block is logically rectangular, or structured (Figure 3.1), and specified as a set of cell corner points, or vertices. The coordinates of the corner points can be in any useful coordinate system: state plane coordinates, for example.

Mesh blocks are logically oriented in the expected flow direction, having an upstream and downstream end and a left and right bank (Figure 3.1). All blocks must have the same orientation, so that when multiple blocks are used, they connect to opposite sides. The downstream edge of one block must connect to the upstream edge of the downstream block, and vice versa. The left bank edge of one block must connect to the right bank of the other block, and vice versa. While this convention is somewhat limiting, it helps to reduce confusion, within both the code and for the user applying the code.

A successful application of MASS2 depends heavily on using an accurate depiction of the bathymetry of the water body. The bathymetry is supplied to MASS2 with the computational mesh. Bathymetry data must be accurate and dense enough to provide the desired resolution. MASS2 also requires a computational mesh of good quality. The key measures of quality are cell orthogonality and aspect ratio. MASS2 can handle small areas of low orthogonality, but most of the mesh should be nearly orthogonal. Cell aspect ratio needs to be low, less than about 1:5 generally, when the cell is oriented along the flow direction. Mesh blocks must also match very closely at block connections. Building a quality curvilinear mesh is a complex task, one which MASS2 does not attempt, so mesh generation software is necessary. For simple applications, the `cartgrid` utility (Section 6.1) can be used to generate Cartesian meshes.

Before building a mesh, it is necessary to determine the mesh boundaries. This is usually based on the expected range of discharge and water surface elevation to be simulated. Where possible, multiple blocks should be used to mesh around dry areas like islands to reduce the computational effort. Sometimes one is tempted build a large mesh that even covers area that will never be inundated. While this makes mesh generation easy, it can greatly increases the computational effort required by the model. Computational effort can also be reduced by concentrating mesh resolution only where needed. Blocks with very fine resolution can be used where simulation results are particularly important or gradients of simulated quantities are large. Coarser blocks can be used elsewhere, extending to locations where boundary conditions are known or easily estimated.

Computational mesh files can be prepared in a variety of ways. The method depends on the preferences of the user, available software, and the available data and its form. The usual method used by the authors involves a geographic information system (GIS) that is to store and manipulate bathymetry data. The GIS is used to build a three-dimensional representation of the river bottom using available data. This may require filtering, interpolation, and smoothing of the original data. A boundary for the mesh is also typically constructed within the GIS, e.g., from shoreline data. The boundary points are exported in a format readable by the Gridgen mesh generation software (Steinbrenner et al. 2000a,b). The mesh generation software is used to generate a mesh, the vertices of which are imported back into the GIS, where each is assigned an elevation from the bathymetry

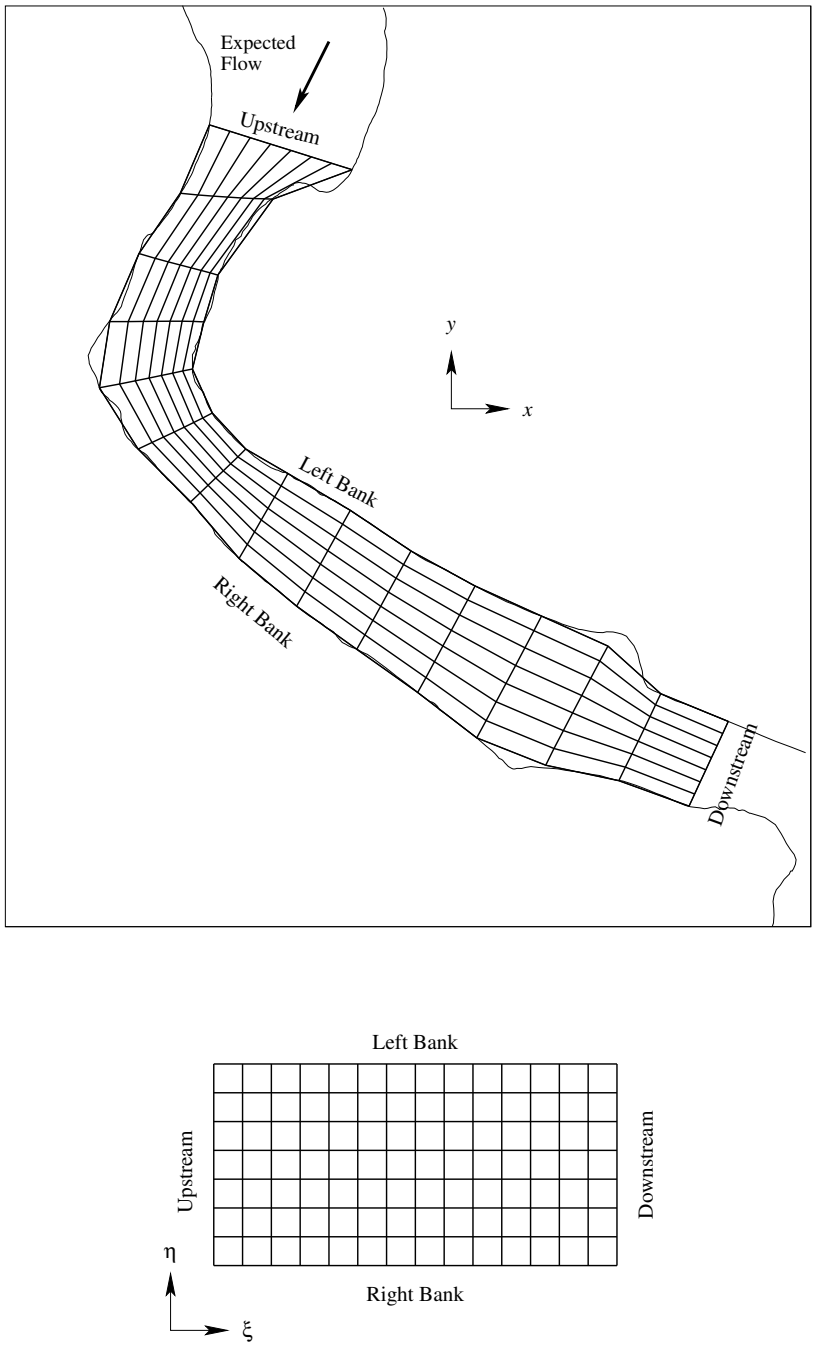


Figure 3.1. Example computational mesh block in physical space (above) and in computational space (below).

surface. The vertices, with their assigned elevations, are then exported from the GIS and formatted for use with MASS2.

3.2 Initial Setup

It is best to configure a MASS2 application in small steps. This section discusses a series of small steps to prepare a MASS2 application. The goal is to ensure that input files were prepared and read properly. Because MASS2 has a complicated input structure (Section 2.3), input preparation can be difficult for the new and experienced user alike.

Start with an existing configuration file named `mass2.cfg`[(a)] and an empty `bc_specs.dat` file (Section 4.3). A configuration file can be prepared from scratch but is usually easier to copy and modify an existing one. Edit the configuration file (refer to Section 4.1 for detailed format information) and do the following:

- Specify the number of blocks (record 3).[(b)]
- Replace the computational mesh file names (record 5) with those to be used the in application.
- Turn both the hydrodynamics (record 6) and transport simulation (record 7) off (`F`).
- Set the start and end time the to be the same (records 15 and 16).
- Turn gage output (record 13) off (`F`).
- Turn two-dimensional output on (`T` in record 39 for NetCDF or record 40 for CGNS).
- Set the reading initial conditions a hot-start file off (`F` in record 11).

This limits MASS2 input to the two required files, `mass2.cfg` and `bcspecs.dat` but does not allow MASS2 to attempt any simulation. No other files should be read, and because `bc-specs.dat` is empty, the reading of `mass2.cfg` is verified. It always best to start with a configuration file known to work and modify and verify it in small steps. When the configuration file is successfully read, MASS2 should report

```
calling mass2_main
Pacific Northwest National Laboratory

mass2 code version 0.27
release: $Date: 2003/05/16 22:43:27 $
completion with status=  1
```

(a) Some examples can be found in Appendix A.
(b) Record numbers will correspond to line number if only one computational mesh block is used.

where the version and date may be different. If some other message is displayed, MASS2 has encountered an error in the configuration file. These are difficult to diagnose, because error messages depend on the compiler used. For example, if MASS2 is compiled with the Absoft compiler under Linux, messages from such errors look like

```
? FORTRAN Runtime Error:
? Illegal character in numeric input
? READ(UNIT=10,...
```

However, if the Intel compiler is used, the messages are somewhat more helpful; for example,

```
  Input/Output Error 137: Value not recognized

   In Procedure: mass2_main_025..read_config
        At Line: 658

      Statement: List-Directed READ
           Unit: 10
   Connected To: mass2.cfg
           Form: Formatted
         Access: Sequential
Records Read   : 52
Records Written: 0

Current I/O Buffer:

1440 F  print_freq  ! printout frequency
        !

End of diagnostics
```

This actually shows the line in the configuration file where the error occurred.

After the configuration file is successfully read, the computational mesh should be checked. MASS2 will have produced a file named `gridplot1.dat` (Section 5.2). Use Tecplot to read this file directly and examine the mesh and the bathymetry assigned to the mesh. An example plot is shown in Figure 3.2. If anything does not look as expected, errors may exist within the computational mesh files. Common errors include wrong block sizes at the top of the mesh file and incorrect ordering of vertices within the mesh file. These will be readily apparent when the mesh is examined.

Once the computational mesh has been verified, the `bcspecs.dat` file can be constructed. Section 4.3 describes the format of the file. The most common configuration is to impose a discharge condition at the entire upstream boundary and a stage condition along the entire downstream boundary. Such a configuration, having a single block, would have two lines in `bcspecs.dat` something like:

```
 1  US TABLE FLUX ALL  "./BCFiles/flow.dat" /
 1  DS TABLE ELEV ALL  "./BCFiles/stage.dat" /
```

When the configuration involves block connections and conditions applied along partial boundaries, it is helpful to use Tecplot with the `gridplot1.dat` to identify connectivity. The cell indexes generated by Tecplot,[(c)] like those shown in Figure 3.2, are the same as those used in `bcspecs.dat`. The block connections shown in Figure 3.2 would be specified as

```
1 DS BLOCK ELEV PART 2 1 14 /
1 DS BLOCK ELEV PART 3 15 19 /
2 US BLOCK VELO ALL  1 /
3 US BLOCK VELO ALL  1 /
```

For complicated domains, it is best to construct `bcspecs.dat` a few conditions at a time. Each time a boundary condition or block connection is added, run MASS2 to verify the contents of `bcspecs.dat`. Block connections are expected to be paired, and an error results if they do not match. Once `bcspecs.dat` is complete, a cold start simulation can be attempted.

3.3 Cold Start

The initial simulation performed in any application is the "cold start." The cold start is used to bring the domain from a crude estimate of initial conditions a more physically reasonable condition, which can then be used to start subsequent simulations. The cold start should be performed with hydrodynamics only. Even if the eventual use of transport or transport-only mode is planned, it is necessary to get the hydrodynamics working first.

Starting with the configuration file and `bcspecs.dat` assembled in Section 3.2, initial conditions must be specified. The specification of initial stage and velocity is a key part of a successful cold start. Two strategies are used for specifying initial conditions. The appropriate strategy depends on the specific problem and available data. The first strategy is to assume that the water surface elevation (or depth) is constant and velocity zero over the entire domain. This strategy is used most often and is particularly good at cold-starting lakes, reservoirs, or estuaries, where water surface slopes are generally low. The initial water surface elevation (or depth) and velocity components are specified in the configuration file (records 33, 30, and 31). In some cases, better information may exist, from another, simpler model, for example, that may provide a more self-consistent initial condition (i.e., depth and velocity correspond with each other). This information can be supplied to MASS2 through the initial profile input (Section 4.7). This strategy is most useful for cold-starting simulations of long, steep channels.

Once initial conditions are chosen, turn the hydrodynamic simulation on (`T` in record 6 of the configuration file) and run MASS2. Start and end times should still be the same, so no simulation will be performed, but the initial hydrodynamic conditions will be written in two-dimensional

(c) In Tecplot 10, for example, plotting of cell indexes can be enabled under the "Label Points and Cells" option of the "Plot" menu.

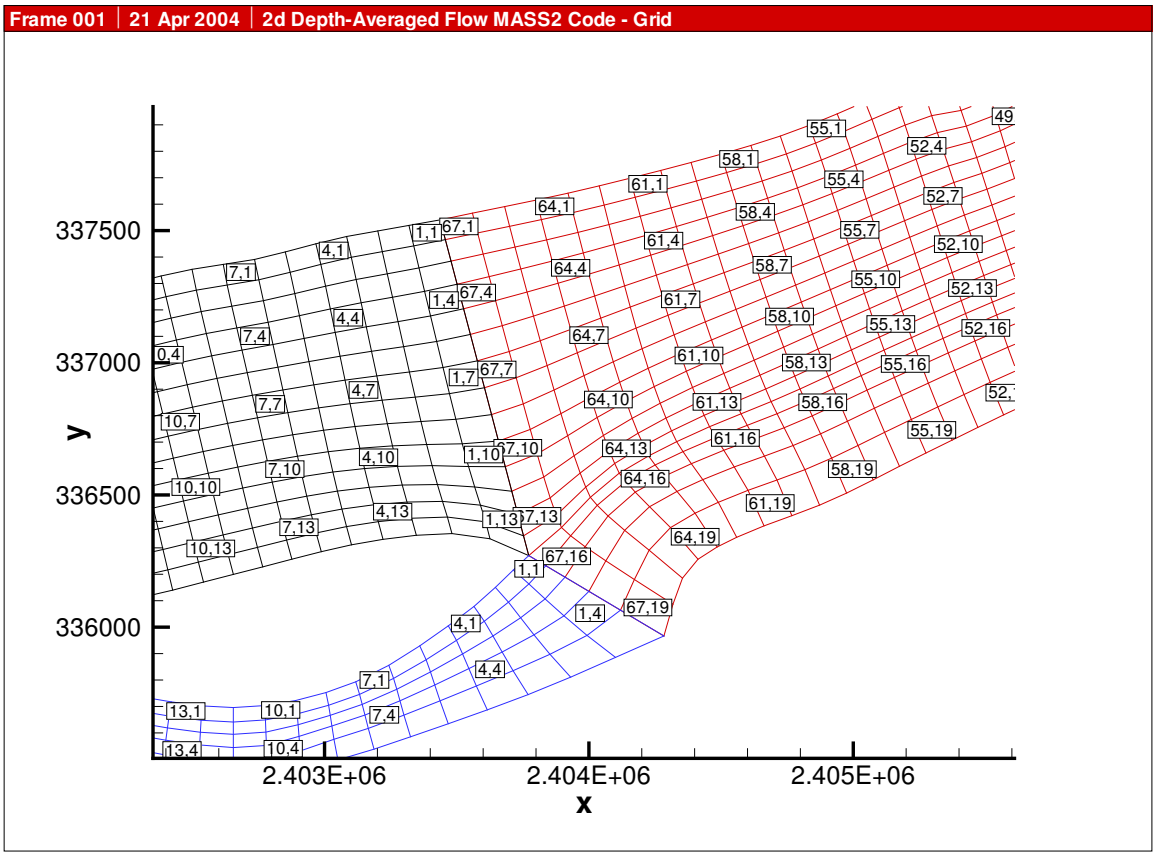


Figure 3.2. Example computational mesh plot generated using Tecplot and the `gridplot1.dat` output file. The blocks shown are oriented with the upstream edge on the right side of the figure and the downstream on the left. Block 1 is red, 2 is black, and 3 is blue. The cell indexes shown were generated by Tecplot and match those used for boundary condition specifications in the `bcspecs.dat` file.

output. These can be examined using Tecplot (see Section 3.7.1) to ensure they were specified correctly.

It is important to consider the relationship between the initial water surface elevation and the boundary conditions to be imposed when the cold start simulation begins. For boundaries where flux or velocity is to be imposed, some cells must be wet, so the initial elevation needs to be above the bottom of at least some of those boundary cells. For boundaries where stage is to be imposed, the initial elevation should be chosen at or near the elevation to be imposed at the boundary. Large differences between imposed stage boundary conditions and initial water surface elevation can cause MASS2 to become unstable rapidly. Usually, the initial elevation and the boundary condition should not differ by more than 1 ft.

Wet and dry areas should also be considered when the initial water surface elevation is chosen. While it is not necessary to have the entire domain be wet initially, it is necessary to select a stage at which there is a reasonable path for flow, particularly at the boundaries. It is usually best to enable wetting and drying even if the domain is not expected to dry. Spurious waves can be generated

during the cold start, often causing negative depths to be simulated. If wetting and drying are enabled, MASS2 can sometimes recover from this situation.

If the initial conditions appear reasonable, a simulation can be attempted. This initial simulation is the most difficult part of applying MASS2 to a given problem. The cold start must converge more slowly to a solution to avoid instability, so MASS2 must be run "gently." Consequently, the configuration of a cold start (e.g., time step, eddy viscosity, hydrodynamics iterations, etc.) will be different from subsequent simulations. While the cold start simulation is usually difficult, subsequent simulations start easily with consistent conditions produced. Good bathymetry, a quality mesh, and reasonable initial conditions will ease the cold start significantly.

Turn gage output on (record 13 of the configuration file) so that the mass source error for hydrodynamics (Section 5.3) is written. It will be necessary to create a `gage_control.dat` file (Section 4.6), but this may be empty.

Run the simulation for one time step by setting the end time to be a little more than the start time in the configuration file. If not successful, recheck stage boundary conditions to be sure they are close to the initial conditions. Very often the cold start will not be successful on the first attempt. Several things can be tried when MASS2 does not work:

- Use smaller time step. In general, a cold start will require a time step about 1/4 to 1/2 (or smaller) of the final simulation.
- Use a larger eddy viscosity. When cold-starting steeper river systems, an eddy viscosity 2 to 3 orders of magnitude larger than the final simulation may be needed.
- Use a lower under-relaxation.
- Use fewer hydrodynamic iterations per time step and fewer inner depth correction iterations.

All of these cause MASS2 to converge more gently (Section 2.5). Run the simulation for a few more time steps and examine the mass source error (Section 5.3). Very large values (several orders of magnitude larger than the overall discharge) may indicate too large a time step or mismatched initial/boundary conditions. The mass source error should show a general decrease over simulation time. Simulation parameters may require further adjustment. Finally, change the simulation end time to allow the simulation to run to convergence (mass source error for all blocks drops below the specified maximum).

In very few cases, a cold start must be done in stages. This might involve cold-starting with a very small time step and a very large eddy viscosity, allowing the simulation to run for only a short period (maybe not even completely converged), then restarting with a larger time step and a smaller eddy viscosity.

3.4 Warm Up

The conditions produced by a cold start can be used to start unsteady simulations if the solution has converged and the conditions are close enough to the initial unsteady boundary conditions. In

most situations, however, a warmup simulation will be necessary to transition from the steady-state of the cold start to the full unsteady conditions.

The warmup simulation will use the hot-start produced by the cold start simulation as initial conditions. The simulation should run about twice as long as it would take a wave to travel from one end of the domain to the other. Simulation parameters can probably be more aggressive than in the cold start, in order to tighten convergence, but more gentle than in the unsteady simulation.

3.5 Simulation

Once the cold start and warmup simulations are successful, subsequent simulations are relatively easy. The main concern shifts from just getting a simulation to run to getting an accurate, stable simulation and doing so in a reasonable amount of time. If a simulation is reasonably stable, its speed can be increased at the expense of accuracy, and vice versa. The speed of the simulation can vary with the choice of hydrodynamic iteration parameters. Table 3.1 shows some hydrodynamic simulation parameters used in several applications performed by the authors and others. These may serve as a general guide when building a new application. Some experimentation with the simulation parameters may be necessary to determine the appropriate balance between accuracy and speed.

For unsteady simulations, one must choose a reasonable maximum mass source error. For a natural river simulation, one typically chooses a value that is about 3 to 5% of the overall discharge. If the selected maximum mass source error is too low, MASS2 will expend a great deal of (probably unnecessary) effort to reach that goal, which can unnecessarily lengthen simulation time. If the selected maximum mass source error is too high, the hydrodynamic solution is never converged quite enough, which can lead to inaccurate solutions or instability.

For unsteady simulations, it is important that the hydrodynamics converge most of the time. The number of hydrodynamic iterations and the mass source error should be monitored. The number of iterations should be few (under 10 in most cases) and should not exceed the specified maximum very often. Additional hydrodynamic iterations are usually required when the boundary conditions vary rapidly over time.

3.6 Special Considerations

3.6.1 Wetting and Drying

The proper configuration of wetting and drying is important to simulate most applications successfully. Three parameters, specified in record 36 of the configuration file, control wetting and drying:

1. *dry depth* — the depth below which a cell is considered dry and (essentially) excluded from the hydrodynamic solution.
2. *re-wetting depth* — the (projected) depth at which a dry cell is allowed to become wet and allowed back in the hydrodynamic solution.

Table 3.1. Hydrodynamic solution parameters used in a variety of past applications, both steady (S) and unsteady (US). These parameters may serve as a general guide. Individual applications may require very different parameters.

							Depth Correction
		Resolution, ft		Time	Iterations		Under-
Application	**Type**	**Lat.**	**Long.**	**Step, sec**	**Inner**	**Outer**	**relaxation**
Bonneville Pool	US	98	159	25.0	15	7	0.40
McNary Pool[(a)]	US	147	330	50.0	15	6	0.40
John Day Pool	US	174	313	50.0	15	6	0.30
John Day Dam Tailwater	S	83	125	30.0	15	10	0.40
The Dalles Dam Tailwater	US	25	49	5.0	30	14	0.40
Hanford Reach[(b)]	US	31	49	16.0	25	12	0.30
Little Goose Pool	US	88	210	50.0	15	7	0.30
Lower Snake River (unimpounded)	S	110	118	20.0	50	5	0.15
Padilla Bay	US	93	95	20.0	25	10	0.40
Mississippi River, Devil's Swamp	S	175	134	40.0		10	0.40

(a) See Appendix B, Section B.1.
(b) See Appendix B, Section B.2.

3. *zero depth* — the depth assigned to cells that are initially dry or have a negative depth during the simulation.

Refer to Section 3.7 of the Theory Manual for more details on the roles these parameters play in the wetting and drying algorithm.

The values of these parameters will vary widely between applications. The dry depth should be as close to zero as possible. The rewetting depth should be slightly larger than the dry depth. The zero depth should be less than the dry depth, usually about half. The actual values of the parameters will depend on the application, the expected results, and the desired accuracy. A large dry depth will make the hydrodynamic solution converge more easily but may remove too much of the domain from the solution (over-estimating dry area). A small dry depth usually increases the likelihood of simulating negative depths but results in a more accurate depiction of dry area. A larger time step, more hydrodynamic iterations, and a lower depth correction under-relaxation are usually required to avoid negative depths. The selected dry depth strikes a balance between the two extremes.

Usually the same parameters should be used through all simulation steps (cold start, warmup, etc.) of the application. It is easy to increase the dry depth but difficult to decrease it from one simulation stage to another.

When wetting and drying is enabled, simulated negative depths do not cause MASS2 to abort the simulation. Instead, depth in the affected cells is set to the zero depth, and computations are allowed to continue. Such occurrences are recorded in `error_warning.out` like this:

```
ERROR: Negative Depth =  -1.354519028538538E-002
    Simulation Time: 10-17-2000          09:27:00
    Block Number =   1
    I,J Location of negative depth = (  11 ,   80 )
ERROR: Negative Depth =  -1.216415655714044E-003
    Simulation Time: 10-17-2000          09:28:00
    Block Number =   1
    I,J Location of negative depth = (  11 ,   80 )
```

where the reported depth is in feet and the location is specified with the cell indexes. These messages should be monitored during the course of a simulation because their presence can indicate instability or inaccuracy when the reported negative depths become large. Small (less than 0.1 ft) negative depths are usually not a problem. Sometimes, especially during a cold start, large (several feet) negative depths occur a few times and the model recovers, but repeated large negative depths indicate instability. In that case, reducing the time step and under-relaxation and increasing the dry depth may be in order.

3.6.2 Supercritical Flow

MASS2 can simulate supercritical flow and transitions between subcritical and supercritical flow (i.e., hydraulic jumps). While MASS2 has this capability, some special consideration is needed when supercritical flow is expected in an application. Simulation of supercritical flow usually requires much smaller mesh spacing in the direction of flow, much smaller time steps, and lower depth correction under-relaxation than subcritical flow.

3.6.3 Transport Simulations

If any scalar transport is to be simulated, it is important to get the hydrodynamics working first. Once a converged hydrodynamic solution is available, transport simulations are relatively easy. It is usually just a matter of turning the transport mode on.

As with the hydrodynamic solution, the transport equations are solved iteratively to account for the interdependence of different scalars and block connections. The primary parameter for the transport solution is the number of scalar (outer) iterations, which is specified in record 19 of the configuration file. Usually, two iterations are adequate for a multi-block domain and a single scalar. Up to five or six iterations may be necessary when several interdependent scalars are simulated.

One must be careful to simulate a long-enough period to avoid biasing the results with the initial conditions. Choose an unreasonable concentration value for initial conditions so that any influence the initial conditions have will be readily apparent. For example, if temperature is simulated, a very low temperature (0°C) could be used as an initial condition and the results of the simulation ignored as long as unreasonably low temperatures existed within the domain.

3.7 Post-Processing

After a successful MASS2 simulation, one usually wants to examine the simulation results. As mentioned in Section 2.6, MASS2 has two forms of output: time series at specified gage locations and complete two-dimensional results. This section describes some ways to examine these results using two software packages: Tecplot, used to visualize two-dimensional output (Section 3.7.1), and gnuplot for time series and profile plots (Section 3.7.2). The authors make extensive use of these two packages; examples of graphics produced are shown through out this document.

3.7.1 Using Tecplot

The authors rely heavily on Tecplot for the display and analysis of two-dimensional output from MASS2. Tecplot is a commercial scientific visualization software package available from Tecplot, Inc.[(d)] Tecplot version 10 and later can read the CGNS format directly using its built-in CGNS reader. A custom loader add-in is used for MASS2 NetCDF output. The general use of Tecplot will not be discussed here. The reader is referred to the Tecplot documentation for further information on the general use of Tecplot.

Once two-dimensional simulation results are read into Tecplot, most plots are relatively simple to make. Typical visualization of MASS2 results includes contour plots of depth, water surface elevation, or transported scalar concentration and velocity vector and streamline plots. These plots are straightforward to create for the experienced Tecplot user.

Handling wet and dry areas when plotting MASS2 results with Tecplot is not as straightforward. In the results, dry cells have a small but positive depth because of the wetting and drying algorithm. To distinguish dry from wet cells, MASS2 includes a dry cell flag. This flag is 1 to indicate a dry cell and 0 to indicate a wet cell. Tecplot can use this flag to hide dry areas in visualizations of MASS2 results. Figure 3.3(a) shows an example of a depth contour plot from a MASS2 simulation. This plot shows all of the cells in the domain. The red lines indicate mesh block boundaries. This plot includes both wet and dry areas. Tecplot has several options for blanking based on a field value. Figure 3.3(b) shows a plot of the same data with value blanking on, with the "entire cells blanked" option. Blanking was enabled when the dry cell flag exceeded 0.5 (halfway between "wet" and "dry"). Figure 3.3(c) shows another plot of the same data with cells "trimmed along the constraint boundary" with the constraint boundary drawn. The authors prefer to use plots such as Figure 3.3(c) to visualize wet and dry areas from MASS2 simulation results.

3.7.1.1 NetCDF Output Loader

To facilitate the reading of two-dimensional NetCDF output, a custom Tecplot add-in titled "MASS2 loader" was coded. This add-in, when installed, is listed in the import data menu (Figure 3.4). When selected, the MASS2 loader asks the user to select a NetCDF file, then displays a dialog to select variables and time slices that are to be imported. The variables in NetCDF output are described in Section 5.4.3. The selected time slices are imported so that a zone represents a single block at a single time. The zones are ordered with all blocks grouped at one time and the blocks in the same order specified in MASS2. For example, output imported from a simulation

(d) Information is available on-line at `http://www.tecplot.com/`.

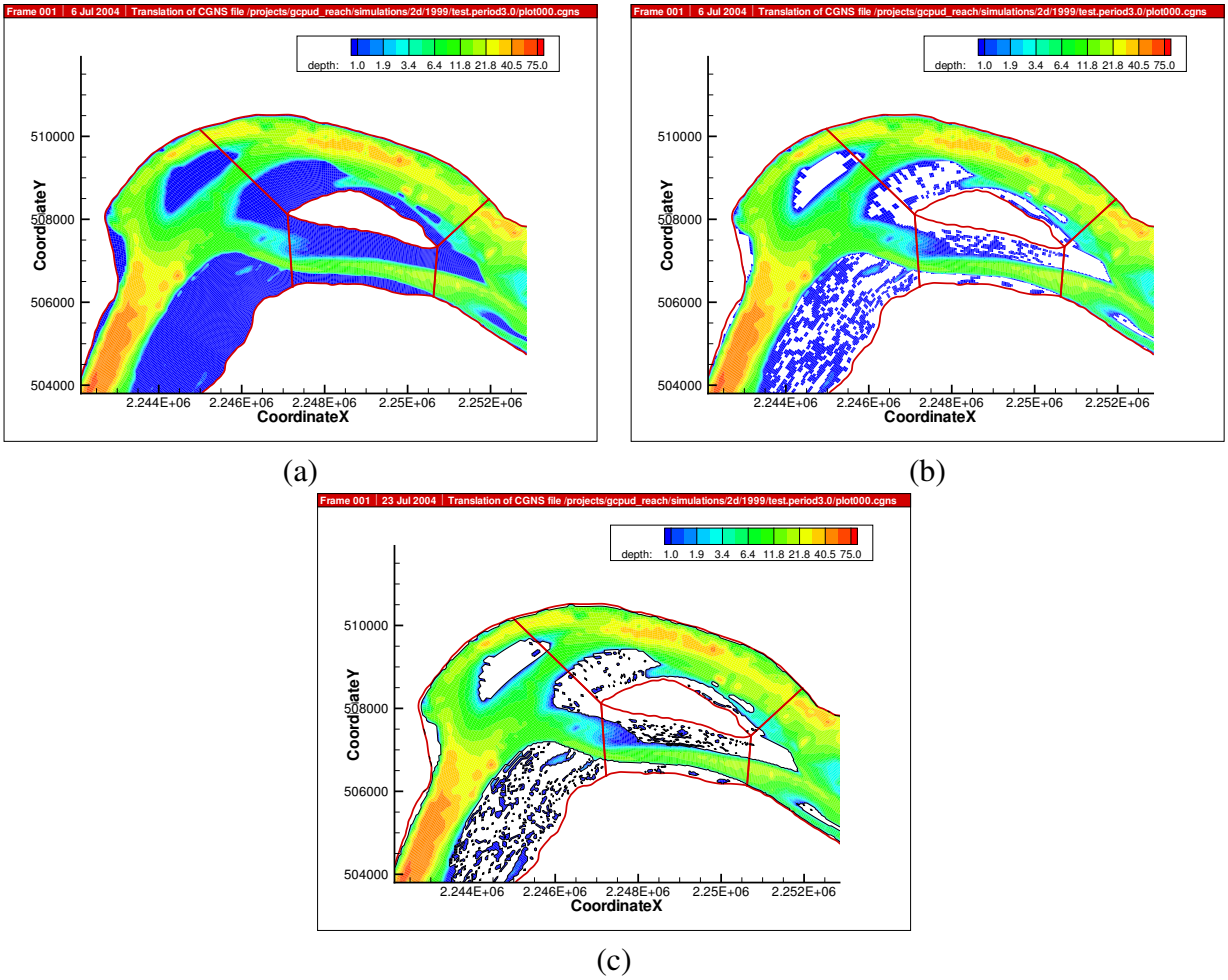


Figure 3.3. Examples of blanking dry areas in Tecplot contour plots: (a) blanking off, (b) blanking when all corners dry, and (c) blanking along constraint boundary with the boundary plotted.

with three blocks and two times will have six zones. The first three zones will be all blocks for the first time, and the second three zones will be all blocks at the second time.

3.7.1.2 CGNS Output Loader

Recent versions of Tecplot have a loader module to read two-dimensional MASS2 CGNS output files directly. The CGNS file to read is specified in the CGNS loader dialog (Figure 3.5). The specified file can be completely or partially imported depending on the specified options. Once imported, data from the CGNS output can be used in the same manner as that from NetCDF output, with two important differences. First, a few variables have different names, as discussed in Section 5.4.4. Second, the CGNS loader orders zones differently than the NetCDF loader. The Tecplot zones will start with all of the time slices for block 1, then all the time slices for block 2, and so on.

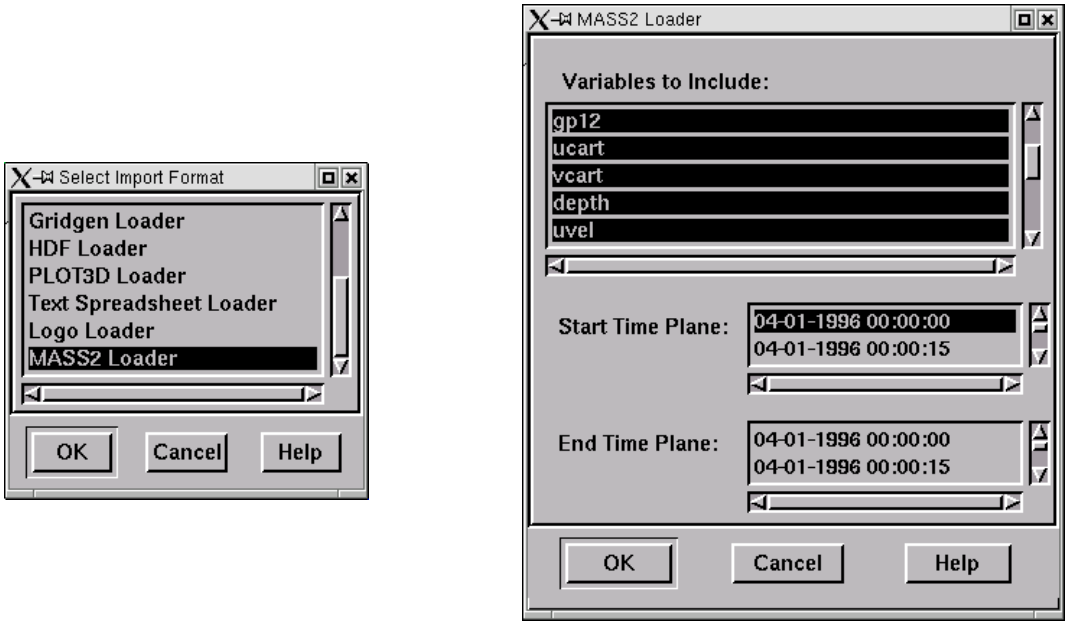


Figure 3.4. Tecplot import dialogs: MASS2 NetCDF loader as an import format choice (left) and the MASS2 loader dialog (right).

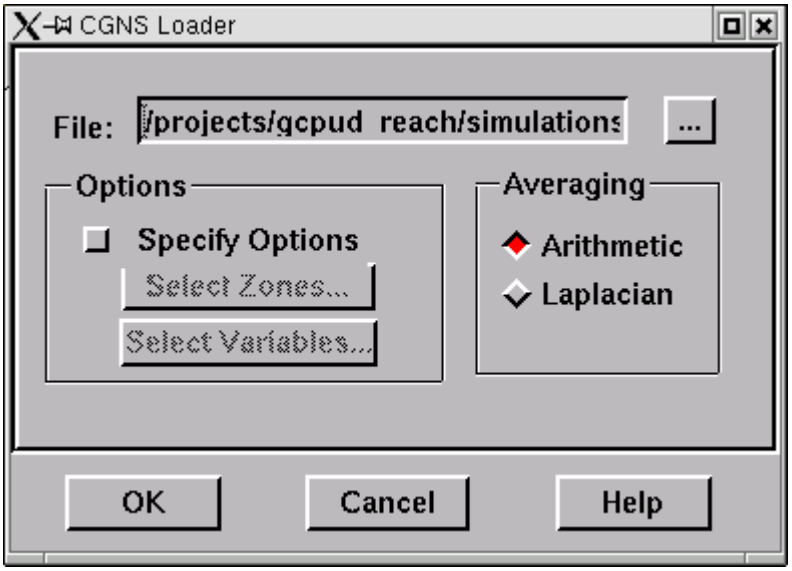


Figure 3.5. Tecplot import dialog for CGNS files.

3.7.1.3 Animation of Multi-Block Grid Output

Animation of MASS2 results is one of the most common tasks for which Tecplot is used. At the time of writing, however, there was no built-in technique for animating a time series of multiple blocks (as there is for a single block domain). Consequently, the animation must be prepared using a macro.

Figure 3.6 shows a Tecplot macro to create an animation from results of a 16 block simulation written to a NetCDF file. The macro loops (starting at line 11) through the time slices and selects a continuous group of zones corresponding to a single time (line 19). When CGNS files are used, the active zones of each animation frame must be determined differently. An example macro for animating MASS2 CGNS output is shown in Figure 3.7. Because of the different zone ordering, the loop starting at line 17 is required to select the appropriate zones.

```
#!MC 800

$!EXPORTSETUP
   EXPORTFNAME = "looper.avi"
   EXPORTFORMAT = AVI
   BITDUMPREGION = ALLFRAMES

$!VARSET |Blocks| = 16
$!VARSET |NLoop| = (|NUMZONES| / |Blocks|)

$!LOOP |Nloop|

$!VARSET |B1| = ((|Loop| - 1)*|Blocks| + 1)
$!VARSET |BN| = (|B1| + |Blocks| - 1)
$!VARSET |MYFRAME| = |Loop|

$!LOOP |NUMFRAMES|
$!FRAMECONTROL PUSHTOP
$!ACTIVEFIELDZONES=[ |B1|-|BN| ]
$!REDRAWALL
$!ENDLOOP

$!IF |MYFRAME| == 1
   $!EXPORT
   APPEND = NO
$!ENDIF

$!IF |MYFRAME| != 1
   $!EXPORT
   APPEND = YES
$!ENDIF

$!ENDLOOP

$!EXPORTFINISH
```

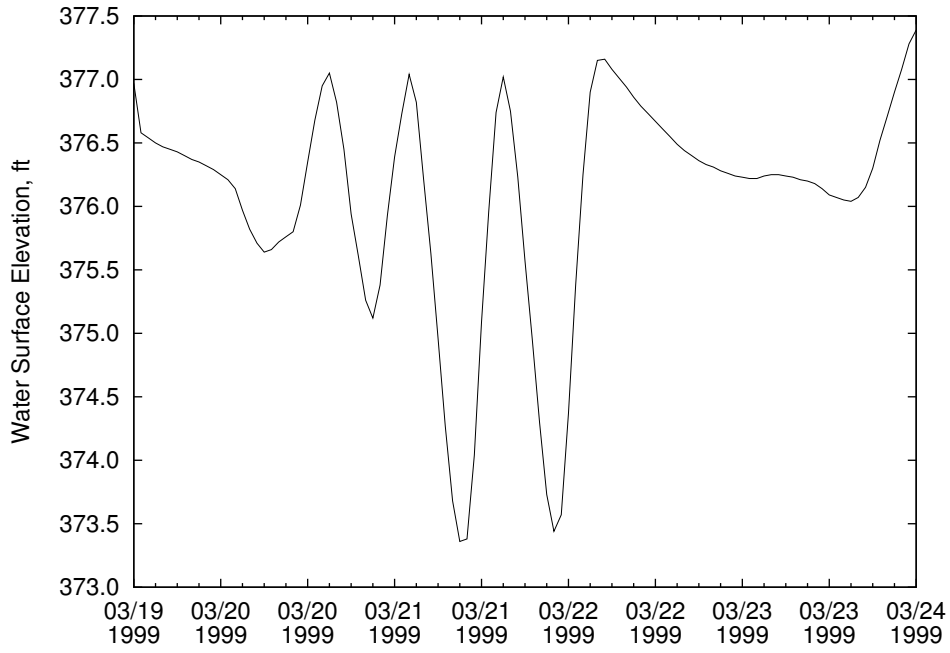
Figure 3.6. An example Tecplot macro to animate NetCDF 2D output.

```
#!MC 800

$!EXPORTSETUP
   EXPORTFNAME = "looper.avi"
   EXPORTFORMAT = AVI
   BITDUMPREGION = ALLFRAMES

$!VARSET |Blocks| = 16
$!VARSET |NLoop| = (|NUMZONES| / |Blocks|)

$!LOOP |Nloop|

$!VARSET |MYFRAME| = |Loop|
$!VARSET |B1| = |Loop|
$!ACTIVEFIELDZONES=[ |B1| ]

$!LOOP |Blocks|
$!VARSET |B1| = (|B1| + |NLoop|)
$!ACTIVEFIELDZONES += [ |B1| ]
$!ENDLOOP

$!LOOP |NUMFRAMES|
$!FRAMECONTROL PUSHTOP
$!REDRAWALL
$!ENDLOOP

$!IF |MYFRAME| == 1
   $!EXPORT
   APPEND = NO
$!ENDIF

$!IF |MYFRAME| != 1
   $!EXPORT
   APPEND = YES
$!ENDIF

$!ENDLOOP

$!EXPORTFINISH
#$
```

Figure 3.7. An example Tecplot macro to animate CGNS 2D output.

3.7.2 Using Gnuplot

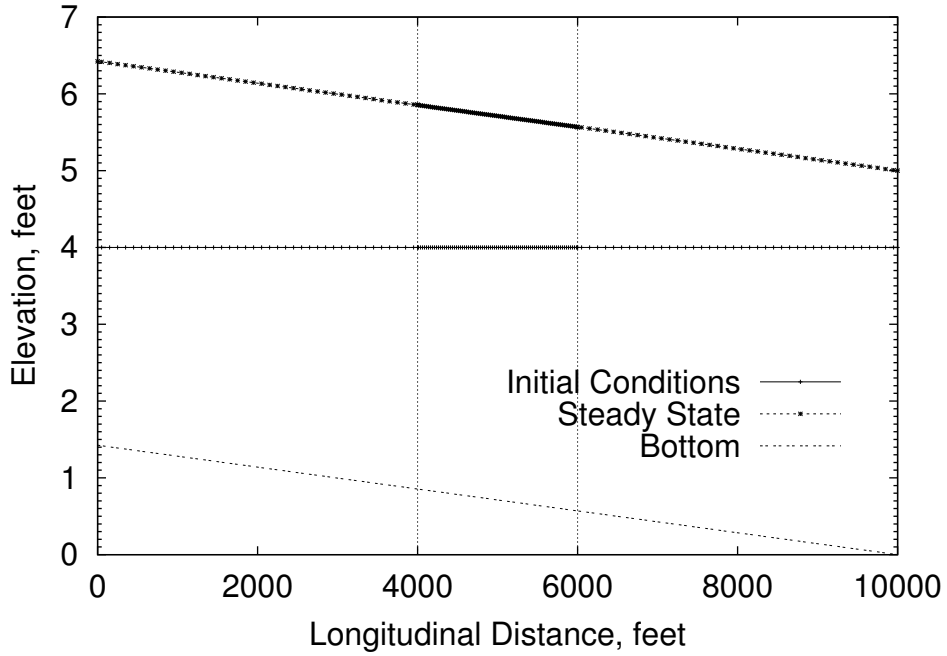
The authors also rely heavily on the freely available plotting software called gnuplot[e] to produce two kinds of graphs from MASS2 output: time series of simulated variables from gage output and profiles of two-dimensional output. To aid in making these plots, the `mass2gage.pl` utility (Section 6.2) is used to extract time series from the gage output file (Section 6.2.1) and the `mass2slice.pl` utility (Section 6.2.2) can be used to extract profiles from NetCDF two-dimensional output (Section 5.4). Figure 3.8 shows an example of using `mass2gage.pl` to make a time series plot of gage data. Figure 3.9 shows an example of plotting a water surface profile from a simulation with three computational mesh blocks.




```
set xdata time
set timefmt '%m-%d-%Y %H:%M:%S'

set format x "%m/%d\n%Y"
set format y "%.1f"
set ylabel "Water Surface Elevation, ft"
set nokey

plot " <perl mass2gage.pl -v wsel -g 10 gage.nc" using 1:3 with lines
```

Figure 3.8. Example time series plot from gage output and the gnuplot script used to make it.

(e) See `http://www.gnuplot.info/` for more information.




```
set ylabel 'Elevation, feet'
set auto y
set xlabel 'Longitudinal Distance, feet'
set mytics
set pointsize 0.5
set key screen 0.8, 0.4

set arrow from first 4000, graph 0.0 to first 4000, graph 1.0 nohead lt 0
set arrow from first 6000, graph 0.0 to first 6000, graph 1.0 nohead lt 0

plot '<perl mass2slice.pl -t 1 -i plot.nc wsel 1 5 2 10 3 5' using 3:4 \
       title 'Initial Conditions' with linespoints 1, \
     '<perl mass2slice.pl -l -i plot.nc wsel 1 5 2 10 3 5' using 3:4 \
       title 'Steady State' with linespoints 3, \
     '<perl mass2slice.pl -i plot.nc zbot 1 5 2 10 3 5' using 3:4 \
       title 'Bottom' with lines 7
```

Figure 3.9. Example gnuplot script to plot a water surface profile.

4.0 Input File Reference

This chapter documents the format of the input files for MASS2. An overview of the MASS2 input structure is presented in Section 2.3. MASS2 input files are plain text and can be prepared using any text editor. MASS2 uses the English system of units internally. Consequently, all input is required to be in English units, except for transported scalar quantities (see Section 4.4).

4.1 `mass2.cfg`: Configuration File

The model configuration is read from a file named `mass2.cfg`. When MASS2 starts, it looks immediately for that file in the current directory and will continue only if the file is found. This file is expected to contain plain text. Each line in the file is considered a record, and each record has as specific number of fields. The file is read using Fortran 90 free-format, so fields are separated by white space. Comments may appear in the record after all of the required fields and they will be ignored. The format of `mass2.cfg` is not very readable or user friendly. A less restrictive and more readable format is being considered for future versions.

The `mass2.cfg` file consists of an ordered series of file name, true/false flags, and parameter values, all of which must be present. Table 3 lists the records of `mass2.cfg`. With the exception of record 5, all records must be on a single line. Record 5 specifies the files containing the computational mesh, which are listed one file name to a line. In record 5 and several others, file names or other text strings are specified. These should be enclosed in double quotes (`"`) when they contain white space or a slash (`/`). Logical switches or flags are specified using "`T`" for true or "`F`" for false.

Table 4.1. Records in the configuration file.

Record	Field	Type	Description
1			Line read and discarded.
2		string	Title of simulation (entire line read).
3	1	integer	Number of computational mesh blocks.
4	1	integer	Number of transported variables. A value is always required and must be greater than zero, but it is only used when scalar transport is enabled in record 7.
5[(a)]	1	string	Name of the file containing a single grid block. The file should have the format described in Section 4.2. If the filename contains spaces or a "/", then the entire name must be in enclosed in double quotes. One line in the file is used for each grid file name. The number of grid files expected is the number of blocks specified in record 3.
6	1	flag	If true, hydrodynamics are simulated.

(a) This record is made up of multiple lines.

Table 4.1. Records in the configuration file (continued).

Record	Field	Type	Description
7	1	flag	If true, scalar transport is simulated, and the files `scalar_source.dat` (Section 4.4) and `scalar_bcspecs.dat` (Section 4.5) are expected to exist in the current directory.
8	1	flag	not used
	2	flag	not used
	3	string	The name of the file from which meteorologic data is to be read (see Section 4.10.3). This file is required to exist if atmospheric exchange is enabled for total dissolved gas or temperature.
9	1	flag	If true, a lot of extra, and usually unintelligible, output is put into `status.out` and `output.out` (Section 5.1).
10	1	flag	If true, bed resistance is computed using Manning's equation; otherwise, the Chezy equation is used. This affects the value supplied in record 25.
11	1	flag	If true, hot-start files (Section 5.6) are written at regular intervals.
	2	integer	The number of simulation time steps between which hot-start files are written.
12	1	flag	If true, initial conditions are read from a hot-start file named `hotstart.bin` created in a previous simulation.
13	1	flag	If true, gage location output (Section 5.5) is enabled and gage location information is read from a file named `gage_control.dat` (Section 4.6). This also enables the output of mass source error (Section 5.3). Gage and mass source error output frequency is set in record 41.
14	1	flag	If true, and initial conditions are not read from a hot-start (record 12, the value supplied in record 33 will be used as the initial water surface elevation over the entire domain; otherwise, the value is used as the initial depth.
	2	flag	If true, initial hydrodynamic conditions are estimated from a precomputed water surface profile. The profile data are read from `initial_specs.dat` (Section 4.7).
15	1	date	Simulation start date in the format described in Section 4.10.1.
	2	time	Simulation start time in the format described in Section 4.10.1.
16	1	date	Simulation end date.
	2	time	Simulation end time.
17	1	real	Simulation time step, sec.
18	1	integer	Maximum number of hydrodynamic (outer) iterations per time step.
	2	real	Maximum mass source error.
19	1	integer	Number of scalar transport (outer) iterations to perform each time step.
20	1	integer	Maximum number of TDMA solver (inner) iterations to perform when solving for momentum and transported scalar equations.
21	1	integer	Maximum number of TDMA solver (inner) iterations to perform when solving the depth correction equation.

Table 4.1. Records in the configuration file (continued).

Record	Field	Type	Description
22	1	real	Default value of eddy viscosity, ft^2/sec.
	2	flag	If true, spatially varying eddy viscosity is read from `eddy_coeff.dat` (Section 4.12).
23	1	real	Default longitudinal (upstream/downstream) diffusivity, ft^2/sec.
	2	flag	If true, spatially varying longitudinal diffusivity is read from `kx_coeff.dat` (see Section 4.12).
24	1	real	Default lateral diffusivity, ft^2/sec.
	2	flag	If true, spatially varying lateral diffusivity is read from `ky_coeff.dat` (see Section 4.12).
25	1	real	Default roughness coefficient. This is either Manning n or Chezy C depending on record 10.
	2	flag	If true, spatially varying roughness coefficient is read from `roughness_coeff.dat`. (Section 4.12)
26	1	real	Coefficient C_o for Manning's equation, either 1.49 for English units or 1.0 for metric units. MASS2 is currently unable to simulate in metric units, so this should always be 1.49.
27	1	real	Depth correction under-relaxation.
28	1	real	Not used.
29	1	real	Not used.
30	1	real	Initial longitudinal velocity used for a cold start, ft/sec. If a hot-start file (record 12) or initial profile (record 14) is read, this value is not used.
31	1	real	Initial lateral velocity used for a cold start, ft/sec. If a hot-start file (record 12) or initial profile (record 14) is read, this value is not used.
32	1	real	Initial scalar concentration used for a cold start, mass/ft^3, where mass is a user-defined mass unit. If a hot-start file (record 12) is read, this value is not used.
33	1	real	Initial water depth or water surface elevation, ft, depending on the first flag in record 14. If a hot-start file (record 12) or initial profile (record 14) is read, this value is not used.
34	1	real	Longitudinal wind speed, ft/sec. This should always be zero.
35	1	real	Lateral wind speed, ft/sec. This should always be zero.
36	1	flag	Enable wetting and drying (Theory Manual, Section 3.7). Enabling wetting and drying will allow cells to dry. Any negative depths simulated will be corrected. Without wetting and drying, cells are not allowed to dry, and MASS2 will abort a simulation in which a negative depth is encountered.
	2	real	The depth below which a cell is considered dry, ft (dry depth).
	3	real	The depth above which a cell is allowed to rewet, ft. This is equal to or greater than the dry depth.

Table 4.1. Records in the configuration file (continued).

Record	Field	Type	Description
	4	real	The initial depth assigned to dry cells, ft (zero depth). If at initialization, the cell depth is less than the zero depth, the cell depth is assigned the zero depth. When a negative depth is simulated, the depth is reset to the zero depth. This should be less than the dry depth.
37	1	real	The bed porosity to be used over the entire domain.
	2	real	The initial bed depth, ft. If no other information is supplied using a hotstart or initial bed files (Section 4.11), the bed is set to this depth, and its composition is assumed to be equally divided among the number of sediment fractions specified in the `scalar_source.dat` file (Section 4.4).
	3	flag	If true, read the initial bed depth and composition from initial bed files (Section 4.11).
	4	integer	Number of sub-time-steps used in the simulation of contaminant bed sources moving through the bed (see Section 3.8.2.2 of the Theory Manual).
38	1	integer	Two-dimensional (plot) output frequency, in time steps. Two-dimensional output, in the format(s) specified in records 39 and 40, is saved repeatedly after the specified number of time steps. Initial conditions and the final simulated state are always saved.
	2	flag	Summarize two-dimensional output. If true, two-dimensional output data is averaged over each output interval instead of the instantaneous state at the end of each output interval (see Section 5.4.2).
39	1	flag	Output NetCDF plot data. If true, two-dimensional output will be written in NetCDF format (Section 5.4.3).
	2	flag	Output hydrodynamic diagnostic variables. If true, any two-dimensional output (both NetCDF and CGNS) will contain diagnostic or derived hydrodynamic variables. These can be computed with the variables in the base hydrodynamic output. Sometimes it is convenient to have the model compute them.
	3	flag	If true, output hydrodynamic variables in transport-only mode.
40	1	flag	If true, output two-dimensional plot data to a CGNS format file (Section 5.4.4).
	2	flag	If true, CGNS output is cell-centered rather than vertex-centered (see Section 5.4.4).
	3	flag	If true, include variable field descriptions in the CGNS file. Older versions of CGNS had problems with too many data nodes in the file. Turning this off can reduce the number of nodes.
	4	integer	Number of time planes written to each CGNS output file; see Section 5.4.4 for details.
41	1	integer	Gage output frequency in time steps. Gage (Section 5.5) and mass source error output are written at the specified frequency if enabled with the flag in record 13.

4.2 Computational Mesh Input Files

The computational mesh is specified using one plain text file for each computational mesh block. The names of these files are specified in record 5 of the configuration file (Section 4.1). Each mesh file is used to specify the size of the block, in terms of the number of downstream and cross-stream vertices (cell corner), and the location and elevation of each vertex in the block's computational mesh. The mesh consists of a list of cell vertices with an elevation assigned to each. The vertices are numbered as shown in Figure 4.1. This file format is also used to supply MASS2 with initial conditions data (Section 4.7) and scalar bed, or non-point, source data (Section 4.9).

The first line of the file contains two fields indicating (1) the number of vertices longitudinally in the block ($i_{\max}$ in Figure 4.1) and (2) the number of vertices laterally in the block ($j_{\max}$) in Figure 4.1). The remainder of the file is expected to have one line for each vertex with five fields, separated by white space, per line:

1. longitudinal index (i)
2. lateral index (j)
3. x, or east, coordinate in physical space, ft
4. y, or north, coordinate in physical space, ft
5. bottom elevation at (x, y), ft.

The first two fields, the indexes, are not used by the model but are there to help the user correctly order the vertices in the file. The vertices must be listed by longitudinal index (i) from the upstream edge to the downstream edge first then lateral index (j) from the right bank to the left bank. MASS2 expects to find a total of $i_{\max} \times j_{\max}$ vertices in the file. If too few are found, an error message is displayed and execution halted. Extra vertices, however, are silently ignored. Each line should be terminated with a "`/`."

Figure 4.2 shows an example of a correct computational mesh input file. In this example, the block mesh contains four vertices longitudinally and five laterally. The total number of vertices supplied is 20. The example has the vertex indexes starting with 0 instead of 1, which is valid because the index fields are arbitrary and only there to aid the user.

4.3 `bcspecs.dat`: Hydrodynamic Boundary Condition Specifications

Hydrodynamic boundary conditions and connections for multiple mesh blocks are specified in a file named `bcspecs.dat`. This file is assumed to be in the current directory and is always required (but may be empty). The file consists of a series of records, each specifying a single condition for a single block. The `bcspecs.dat` file is plain text and is read using free-format Fortran 90. Fields are separated by white space, and each record must be terminated with a "`/`." If a field contains white space or a "`/`," it must be placed between double quote marks (`"`). An example `bcspecs.dat` file is shown in Figure 4.3.

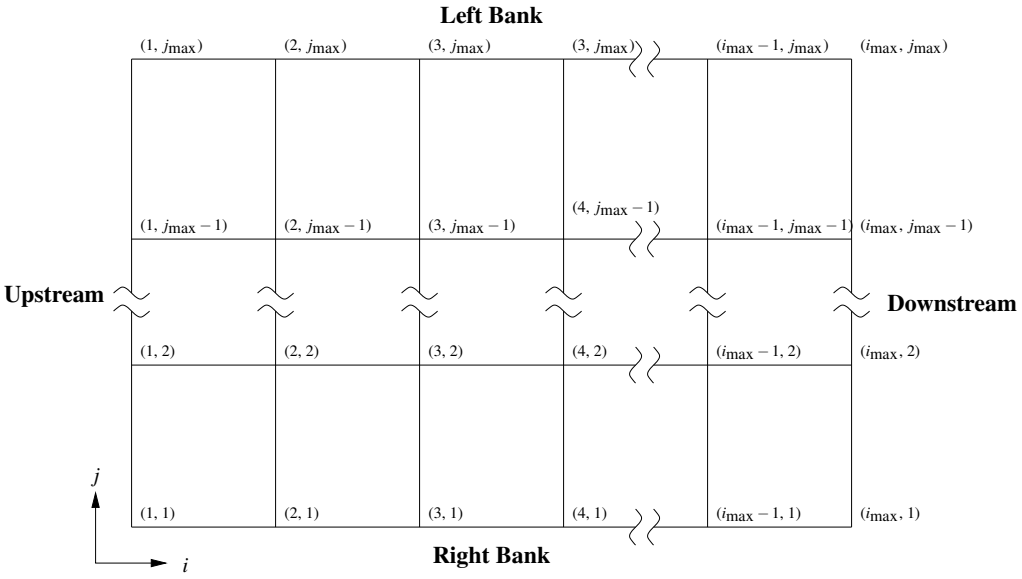


Figure 4.1. Mesh block vertex indexing used in computational mesh input files. The files are expected to list the vertices in row (i) order.

```
    4     5
    0     0     2245623.000     507934.375     373.938 /
    0     1     2245408.250     508039.062     372.142 /
    0     2     2245193.500     508143.750     372.973 /
    0     3     2244978.750     508248.438     373.997 /
    0     4     2244764.000     508353.125     374.704 /
    1     0     2245711.000     508504.156     372.800 /
    1     1     2245614.750     508566.531     370.826 /
    1     2     2245514.250     508630.812     371.178 /
    1     3     2245407.750     508696.875     372.848 /
    1     4     2245291.250     508766.969     374.213 /
    2     0     2246111.000     508914.594     373.445 /
    2     1     2246025.250     508995.250     372.007 /
    2     2     2245940.750     509073.562     370.003 /
    2     3     2245856.500     509151.656     369.722 /
    2     4     2245769.750     509232.125     372.915 /
    3     0     2246594.000     509233.312     373.184 /
    3     1     2246485.000     509362.688     369.793 /
    3     2     2246376.250     509492.062     366.056 /
    3     3     2246267.250     509621.406     364.946 /
    3     4     2246158.500     509750.781     373.231 /
```

Figure 4.2. Example of a computational mesh input file.

```
 1 US TABLE FLUX PART "BC Files/JDA_QS.prn"  1 10  /
 1 US TABLE FLUX PART "BC Files/JDA_QP.prn" 11 24 /
 1 DS BLOCK ELEV PART  2 1 9 /
 1 DS BLOCK ELEV PART  3 10 24 /
 2 US BLOCK VELO ALL   1 /
 2 DS BLOCK ELEV ALL   4 /
 3 US BLOCK VELO ALL   1 /
 3 DS BLOCK ELEV ALL   4 /
 4 US BLOCK VELO PART  2  1  9 /
 4 US BLOCK VELO PART  3 10 24 /
 4 DS BLOCK ELEV PART  5  1  8 /
 4 DS BLOCK ELEV PART  6  9 24 /
 5 US BLOCK VELO ALL   4 /
 5 DS BLOCK ELEV ALL   7 /
 6 US BLOCK VELO ALL   4 /
 6 DS BLOCK ELEV ALL   7 /
 7 US BLOCK VELO PART  5  1  8 /
 7 US BLOCK VELO PART  6  9 24 /
 7 DS BLOCK ELEV PART  8  1 15 /
 7 DS BLOCK ELEV PART  9 16 24 /
 8 US BLOCK VELO ALL   7 /
 8 DS BLOCK ELEV ALL  10 /
 9 US BLOCK VELO ALL   7 /
 9 DS BLOCK ELEV ALL  10 /
10 US BLOCK VELO PART  8  1 15 /
10 US BLOCK VELO PART  9 16 24 /
10 DS TABLE ELEV ALL "BC Files/TDA_FBZ.prn" /
```

Figure 4.3. An example of the `bcspecs.dat` input file

The number of fields and their expected content vary depending upon the type of condition and where it is to be applied (Table 4.2). The first field of the record is always the block number. Blocks are numbered consecutively as they are listed in the configuration file (record 5) starting with 1. The second field is a code indicating where the boundary condition is to be applied. The codes `US`, `DS`, `RB`, and `LB` refer to the block's upstream, downstream, left bank, and right bank sides and indicate an open boundary condition, discussed in Section 4.3.1, or block connection, discussed in Section 4.3.2. The code `IN` indicates an internal condition, which is discussed in Section 4.3.3. If no condition is specified for a block side, it is assumed to be a zero flux boundary.

4.3.1 Open Boundary Condition Specification

Open boundaries are specified where conditions are known. Two kinds of conditions can be specified by using the keyword `TABLE` or `ZEROG` in the third field of the record. The `TABLE` keyword indicates that a time series of values is to be applied. The `ZEROG` keyword indicates that a zero gradient condition is to be applied at the boundary for both velocity components and the depth correction.

Table 4.2. Acceptable key words by record type in `bcspecs.dat`. All allowable words are listed, but certain combinations are not supported or not allowed (see text for details). Where "*file*" appears, a file name is expected. An integer index is expected where *block*, *index1*, *index2*, etc., appear.

Field 1	Field 2	Field 3	Field 4	Remainder
			Open Boundary Conditions	
block	US	TABLE	FLUX	ALL "*file*"
	DS		VELO	PART "*file*" *index1 index2 ...*
	RB		ELEV	
	LB		ELEVEL	
block	US	ZEROG	(ignored)	ALL
	DS			PART *index1 index2 ...*
	RB			
	LB			
			Block Connections	
block	US	BLOCK	VELO	ALL
	DS		ELEV	PART *index1 index2 ...*
	RB			
	LB			
			Internal Boundary Conditions	
block	IN	WALL	UVEL	*i jmin jmax*
			VVEL	*j imin imax*
block	IN	DEAD	CELL	*imin imax jmin jmax*
block	IN	SOURCE	FLUX	ALL "*file*"
		SINK	VELO	PART "*file*" *imin imax jmin jmax*

The fourth field is a keyword indicating the type of boundary condition to be applied. This must be present for `ZEROG` records, but is ignored. For `TABLE` records, the keyword defines the what boundary value the time series contains and must be one of the following:

- `FLUX`, for total discharge across the block face
- `VELO`, for velocity normal to the block face
- `ELEV`, for water surface elevation at the block face
- `ELEVEL`, for both water surface elevation at and velocity normal to the block face.

The fifth field is either `ALL` or `PART` meaning that the boundary condition is to be applied over the entire block face or only to a few cells along part of the block face. For `TABLE` records, the next field is the name of the file containing a time series of boundary values, the format of which is described in Section 4.10. If the file name contains white space or a "`/`", it must be enclosed in double quotes (`"`). The file name is omitted for `ZEROG` records.

If the condition is to be applied only on part of the block face (with PART), the remainder of the record is expected to be a list of cell index pairs (up to 10 pairs are allowed). Each pair indicates the portion of the block face to which the boundary condition is to be applied with a starting and ending index. The indexes are inclusive. The file specified in TABLE records must contain one value per time for each index pair. If the ELEVEL condition type is specified, two values, elevation and velocity, in that order, are expected for each index pair.

When discharge (FLUX) or velocity (VELO) conditions are specified, positive fluxes or velocities are inward on upstream or right bank block sides and outward downstream and left bank sides. Water surface elevation (ELEV or ELEVEL) can only be specified on downstream or left bank sides of the block. More information about boundary conditions can be found in Section 3.5 of the Theory Manual.

In the example bcspecs.dat shown in Figure 4.3, open boundary conditions are applied at the upstream and downstream ends of the domain. At the upstream end, two different discharge time series are applied to different portions of the boundary (lines 1 and 2). At the downstream end, a time series of water surface elevations is applied along the entire face of the downstream block (line 27).

4.3.2 Block Connections

The edge of one mesh block can connect to another, either in whole or part. The connections are specified in bcspecs.dat by using the BLOCK keyword in the third field. The fourth field of a BLOCK record indicates the type of connection used, either VELO for velocity, or ELEV for water surface elevation. This keyword has no effect because the actual condition applied is determined internally. However, it may be used in the future when more arbitrary block connections are allowed. The sixth field is either ALL or PART, indicating whether the entire or only part of the block face is involved in the connection. The following field is the number of the connecting block. If PART is used, the remainder of the record contains an index pair indicating the starting and ending indexes of the cells involved in the connection. Several examples of block connection records are shown in Figure 4.3.

The downstream end of a block can only connect to the upstream end of another block, and vice versa. Similarly, the right bank side of a block can only connect to the left bank side of another block, and vice versa. There must be two records for each connection, one for each block. To avoid problems, block connections are checked for consistency. There must be two matching records for each block connection, one for each block involved. Each cell on the coarse side of the connection must correspond to an integral number of cells on the other side. A block connection is also checked to make sure that one side of the connection matches the other side in physical space as well. This is done by comparing the locations of the mesh vertices at each end of the connection and making sure they close (the vertex locations are allowed to about 1% of a cell width apart).

4.3.3 Internal Boundaries

Three kinds of internal boundaries can be specified in the bcspecs.dat file: walls, dead zones, and sources (or sinks). Walls block flow along the edge of a set of cells, either longitudinally

or laterally. Dead zones remove blocks of cells from the solution. Sources provide a mechanism to represent sources of water mass from or to the bed, such as seepage.

A wall is specified by using the keyword `WALL` in the third field. The fourth field indicates the orientation of the wall: `UVEL` blocks longitudinal (upstream/downsteam) flow and `VVEL` blocks lateral (left/right bank) flow. The remainder of the record contains three integer indexes that locate the wall. The first is the cell index for the row or column: *i* for `UVEL`, *j* for `VVEL`. The other two define the start and end cell indexes along that row or column. For example, in this wall specification

```
1 IN WALL  UVEL 73 1  6 /
```

a wall is placed in block 1 along the downstream side of the first six cells of row 73. When a wall is specified, the scalar diffusion across that face is set to zero, so there can be no scalar flux across that face.

Dead zones are specified using the keyword `DEAD` in the third field. The fourth field should always contain the keyword `CELL`. The remainder of the record consists of four indexes defining a rectangular block of cells: $i_{\min}$, $i_{\max}$, $j_{\min}$, and $j_{\max}$. All of the cells falling within the index ranges are set to the specified initial conditions, and their depths are not allowed to change. For scalar transport, dead zone cells are essentially removed from the solution. This is done by forcing the advective and diffusive fluxes in and out of the cell to zero.

If any dead zones are specified, a flag called `isdead` will placed in the two-dimensional output (Section 5.4). This flag can be used like the dry flag as described in Section 3.7.1.

A water source (sink) can be specified by using the `SOURCE` (`SINK`) in the third field of the record. The source can be specified as a total flux or as a flux per unit area by using `FLUX` or `VELO` in the fourth field. The fifth field is either `ALL` or `PART`. The name of the file containing the source time series is specified in the sixth field. The remainder of the record contains four indexes defining a rectangular block of cells as with dead zones.

The time series file contains a flux in ft^3/sec, or a flux per unit area in ft/sec. A flux is divided evenly among the active cells in the specified range. The keyword `SINK` indicates that positive rates in the time series are *outflow* rates.

4.4 `scalar_source.dat`: Transported Scalar Properties

The `scalar_source.dat` is used to define the properties of the transported scalar quantities to be simulated. The file is plain text and must have a single record for each transported scalar quantity, the number of which is specified in record 4 of the configuration file. The file is read with free-format Fortran 90, so each record is terminated with a "`/`" and may span multiple lines. The fields within a record are separated with white space. Fields containing a "`/`" and/or white space must be enclosed in double quotes (`"`).

The first five fields are the same for any scalar type (Table 4.3) and are required (Table 4.4). The first field is an integer identifier. The identifier must be between 1 and the number of scalars (inclusive), but records need not be in that order. The second field is a keyword that specifies the type of scalar quantity. The third, fourth, and fifth fields are strings descriptive of the scalar quantity: short name, description, and units.

The remainder of each record is made up of keyword/value pairs. The keywords vary with the scalar type and are almost always followed by one or more values corresponding to the keyword. Valid keywords are described in Table 4.4. The keyword/value pairs may appear in any order within the record.

One keyword is common to most transported scalars: `CONVERT`. Internally, MASS2 must use concentration units of mass per ft^3. The value specified by `CONVERT` is used to convert the concentration units of boundary conditions, with user-defined units, to the internal units. It is also used to convert the concentrations from the internal units back to the user-defined units for output. It is only necessary to convert the volume units because MASS2 does not alter the mass units. For example, if the concentration of a transported scalar is to be reported in pCi/L, the value specified with `CONVERT` would be that necessary to convert the concentration to pCi/ft^3: 28.32 L/ft^3.

Some special consideration needs to be given when interdependent scalars are specified. Particulate scalars should use the same units as the dissolved phase. The units for the particulate partition coefficients (`KD` and `BEDKD`) should be the reciprocal of the sediment units. When total dissolved gas is simulated, temperature must also be specified. If `AIREXCH` is specified for either, the meteorology file specified in record 8 is read and used to determine atmospheric exchange.

An example `scalar_source.dat` file is shown in Figure 4.4. In this example, an isotope of Neptunium is to be simulated in two phases, dissolved and particulate sorbed to a single sediment fraction. There is also a non-point source for dissolved Neptunium, which includes a water flow component.

Table 4.3. Keywords used to identify scalar type in the `scalar_source.dat` input file.

Scalar Type	Keyword
Generic, dissolved scalar	`GEN`
Particulate-sorbed scalar	`PART`
Sediment	`SED`
Temperature	`TEMP`
Total dissolved gas	`TDG`

Table 4.4. Records in the `scalar_source.dat` input file.

Record Type	Field or Keyword	Value Description	Default
all	1	Integer used to identify the scalar in other input, like `scalar_bspecs.dat`. These are also used internally as array indexes, so the integers used must be consecutive and less than or equal to the number of scalars specified in the configuration file.	none
	2	Keyword for transported scalar type (see Table 4.3)	required
	3	Short name of scalar. This is used to uniquely identify the scalar in output.	required
	4	Description of scalar. This is used only as documentation in the output. The content of the string does not affect simulation.	required
	5	A string describing the units used in input and output of concentration values. This is used only as documentation in the output. The content of the string does not affect simulation.	required
	`CONVERT`	A real value used to convert from user-defined concentration units to mass/ft^3 used in MASS2 (see text).	1.0
`GEN`	`HALFLIFE`	The half-life of transported scalar, years	0.0
	`BEDSOURCE`	Specify a bed, or non-point, source. If this keyword appears in a record, two arguments are expected. The first is the name of a file containing a list of source time series. The second is the name of a file containing the mapping of the sources time series to the domain. See Section 4.9 for details.	none
	`BEDFLOW`	Specify the water flow part of a bed, or non-point, source. If this keyword appears in a record, two arguments are expected. The first is the name of a file containing a list of source time series. The second is the name of a file containing the mapping of the sources time series to the domain. See Section 4.9 for details.	none
	`DIFFUS`	Diffusivity of the scalar between the water column and bed pore water, ft^2/sec	0.0
`PART`	`DISSOLVED`	Integer identifier for the dissolved phase scalar.	required
	`SEDIMENT`	Integer identifier for the sediment fraction to which this particulate is sorbed.	required
	`KD`	Partition coefficient in the water column, reciprocal of sediment concentration units.	required
	`BEDKD`	Partition coefficient in the bed, reciprocal of sediment concentration units.	required

Table 4.4. Records in the `scalar_source.dat` input file (continued).

Record Type	Field or Keyword	Value Description	Default
	RATE	Rate of exchange between dissolved and particulate phase in the water column, 1/sec.	0.0
SED	D50	Median particle diameter, ft	required
	DENSITY	Sediment solids density, in mass/ft^3, where *mass* is the same mass units used for concentration.	required
	SETVEL	Sediment particle velocity, ft/sec.	required
	DSHEAR	Critical shear stress for deposition, lbf/ft^2	required
	ESHEAR	Critical shear stress for erosion, lbf/ft^2	required
	ERODIBILTY	Erodibility coefficient, *mass*/ft^2/sec, where *mass* is the same mass units used for concentration.	0.0
TEMP	AIREXCH	No value required. If keyword present, atmospheric heat exchange (Theory Manual, Section 2.3.4) is enabled.	disabled
TDG	AIREXCH	No value required. If keyword present, atmospheric gas exchange (Theory Manual, Section 2.3.5) is enabled.	disabled
	PARAMETERS	Name of a file containing the atmospheric exchange coefficients (Section 4.13). Required if AIREXCH enabled.	none

```
1 SED "sediment" "Suspended Sediment" "kg/m^3"
    CONVERT 0.028317
    DENSITY 75.04
    D50  0.0001
    SETVEL      3.3e-05     DSHEAR  1.5e-03
    ERODIBILTY  0.0         ESHEAR  1.5e-03 /
2 GEN "Np237" "Neptunium-237" "Ci/m^3"
    CONVERT 0.028317
    HALFLIFE 2140000.
    DIFFUS   1e-07
    BEDSOURCE  "Np237-list.dat"   "cfestmap.dat"
    BEDFLOW    "bedflow-list.dat" "cfestmap.dat" 35.315 /
3 PART "Np237-part" "Neptunium-237 (Particulate Phase)" "Ci/m^3"
    CONVERT 0.028317
    DISSOLVED 2
    SEDIMENT 1
    KD    0.1000000
    BEDKD 0.1000000
    RATE 1.0E-08 /
```

Figure 4.4. An example `scalar_source.dat` file.

4.5 scalar_bcspecs.dat: Transported Scalar Boundary Conditions

The scalar_bcspecs.dat file is used to specify external boundary conditions for transported scalar quantities. The format of scalar_bcspecs.dat is very similar to bcspecs.dat (Section 4.3). Each boundary condition is specified with a single record having multiple fields separated by white space and terminated by a "/." If any field contains white space or a "/," it must be enclosed in double quotes ("). An example scalar_bcspecs.dat file is shown in Figure 4.5.

The first field is the block number. The second field is a code indicating the block face where the condition is to be applied (codes are the same as in bcspecs.dat). The third field is either TABLE or ZEROG, indicating a user-defined boundary value or a zero-gradient condition. The fourth field is the scalar identifier. This corresponds to the identifier assigned to the scalar in scalar_source.dat. The fifth field is always CONC. The remainder of the record specifies the location of the condition and the boundary value time series file for TABLE records and is the same as bcspecs.dat. Those conditions specifying a TABLE require that the cell row/column at which the condition is to be applied. The use of this feature is discouraged because it has not been tested in recent versions. So, the cell row/column index should always be 1. Eventually, this option will be removed.

If no condition is specified for an open boundary face (not connected to another block), a zero gradient condition is applied. Historically, block connection language was also required, but in the current version of MASS2, block connections are only specified in bcspecs.dat (Section 4.3.2). The old language is allowed but will be ignored.

```
47 US TABLE 1 CONC ALL  "bc/PRD-sediment.dat" 1 /
53 DS ZEROG 1 CONC ALL    /
47 US TABLE 2 CONC ALL  "bc/PRD-Np237-diss.dat" 1 /
53 DS ZEROG 2 CONC ALL    /
47 US TABLE 3 CONC ALL  "bc/PRD-Np237-part.dat" 1 /
53 DS ZEROG 3 CONC ALL    /
```

Figure 4.5. An example scalar_bcspecs.dat file.

4.6 gage_control.dat: Gage Reporting Locations

MASS2 can be made to output time series of simulated conditions at individual locations (or gages). The gage output frequency can be different than the two-dimensional output. This is useful for comparing simulated time series to observations from a gage or instrument at a known locations.

The flag in record 13 of the configuration file must true to enable gage data output. If gage output is enabled, the file gage_control.dat must exist in the current directory (but may be empty). This file is expected to be plain text and is read using free-format Fortran 90. Three fields are expected in each record and a fourth field is optional. Fields are separated by white space, and each record must be terminated with a "/." The fields are

1. grid block number
2. longitudinal cell index (i)
3. lateral cell index (j)
4. location identifier string.

The last field is optional and must be enclosed in double quote marks (") if it contains any white space or a "/." If the last field is not included, the default location identifier string is `block=##i=###j=###`, where `##`s are replaced with the specified block number, i, and j in that order. An example file is shown in Figure 4.6.

Typically, one will know the geographic coordinates of a monitoring location in a geo-referenced coordinate system such as state plane coordinates. The simplest way to identify the cell indexes for `gage_control.dat` is to use Tecplot and the `gridplot1.dat` output file (Section 5.2). With `gridplot1.dat` loaded into Tecplot, the "data probe" tool can be used to find a zone value at a specific location (e.g. cell indexes i and j). Usually, the location is entered using the mouse, but it can also be entered using coordinates if the "Tool Details" button is pressed. The "Zone/Cell Info" panel of the data probe will show what block and cell the location lies in; these indexes can be used in `gage_control.dat`.

Any number of gage locations may be specified. If gage output is enabled, a NetCDF file named `gage.nc` is created in the current directory (Section 5.5). The frequency at which simulation results are saved is set on record 41 of the configuration file.

```
1 16 2          IHRNLGWQ5P /
1 14 16         IHRNLGWQ2P /
1 45  3         MCN00895P /
1 45  7         MCN00894P /
4 48 1          "Fixed Monitor IDSW" /
4 48 4          MCN00615P /
4 48 9          MCN00612P /
4 47 14         MCN00611P /
7 19 2          MCN00221P /
7 19 7          MCN00223P /
7 20 16         MCN00225P /
9 23 2          MCN32355P /
9 23 8          MCN32354P /
9 23 19         MCN32352P /
9 23 22         MCN32351P /
8 41 11         MCN32613P /
13 1 28         MCN31422P /
13 307 10       FMS_MCQW /
13 307 26       FMS_MCQO /
```

Figure 4.6. An example `gage_control.dat` input file.

4.7 `initial_specs.dat`: Initial Water Surface Elevations

MASS2 requires an initial water surface elevation (or depth) and velocity to begin simulation. Typically, these are supplied in the configuration file (records 14, 33, 30, and 31). This approach is adequate to start most applications. In some cases, however, it is helpful to develop cold start initial conditions outside the model, with, for example, a simpler model.

If the second flag of record 14 in the configuration file is true, the file `initial_specs.dat` must exist and have one record for each grid block. An example is shown in Figure 4.7. Each record in the file must contain the name of a file containing the initial water surface elevation to be used for the block. Optionally, two more file names can be supplied in the record, indicating the source of eastward and northward Cartesian velocity components. Each record must be terminated with a "`/`." If the file name for the eastward velocity component is not present in the record or is `NONE`, longitudinal velocities are estimated from the water surface elevations as described in the Theory Manual, Section 3.4. If a file for eastward velocity is present, one for northward velocity must also be present.

The stage and velocity files indicated use the same format as those used to specify the computational mesh block (Section 4.2) with the last field being water surface elevation or velocity instead of bottom elevation. This supplies a value of water surface elevation and velocity at each grid vertex. The the vertex values are averaged to obtain a cell center value. Velocity components are then transformed to the computational coordinate system and averaged to supply lateral and longitudinal velocity components at the appropriate control volume center.

The use of `initial_specs.dat` is a mechanism to provide MASS2 an *approximate* initial condition. This should not be used to restart as simulation using MASS2 results. A hot-start file (Section 5.6) should be used for that.

4.8 `transport_only.dat`: Hydrodynamic for Transport-Only Mode

The transport-only simulation mode (Section 2.2) is enabled when transport is on (configuration file record 7) and hydrodynamics is off (configuration file record 6). In that case, a file named `transport_only.dat` is expected to exist in the current directory. An example is shown in Figure 4.8. The file contains a list of hot-start files (Section 4.14) from which the hydrodynamic conditions for the simulation are read. The `transport_only.dat` is plain text and is read with free format Fortran 90. Each record should be terminated with a slash (`/`) and fields separated with white space. Each record is expected to have three fields: (1) date, (2) time, and (3) the name of a hot-start file (Section 4.14) from which the hydrodynamics for the specified date and time will be read. The date and time should be in the format described in Section 4.10.1.

4.9 Scalar Bed Source Data Files

A scalar bed source is used to represent a non-point source of contaminant that is independent of the hydrodynamics and can vary over the domain. The source is specified as one or more time-varying contaminant mass fluxes. This flux is divided, with user-specified proportions, over one or

```
"Initial/p50b-pt.000"   /
"Initial/p50b-pt.010"   /
"Initial/p50b-pt.009"   /
"Initial/p50b-pt.011"   /
"Initial/p50b-pt.001"   /
"Initial/p50b-pt.002"   /
"Initial/p50b-pt.003"   /
"Initial/p50b-pt.004"   /
"Initial/p50b-pt.005"   /
"Initial/p50b-pt.006"   /
"Initial/p50b-pt.007"   /
"Initial/p50b-pt.008"   /
"Initial/p50b-pt.013"   /
"Initial/p50b-pt.014"   /
"Initial/p50b-pt.012"   /
"Initial/p50b-pt.015"   /
```

Figure 4.7. Example initial_specs.dat file for an application with 16 mesh blocks. In this example, only water surface elevation is specified. In this case, initial velocities would be estimated from the specified water surface elevations.

```
01-15-1998 00:00:00 "hotstart_01-15-1998_000000.bin" /
02-15-1998 00:00:00 "hotstart_02-15-1998_000000.bin" /
03-15-1998 00:00:00 "hotstart_03-15-1998_000000.bin" /
04-15-1998 00:00:00 "hotstart_04-15-1998_000000.bin" /
05-15-1998 00:00:00 "hotstart_05-15-1998_000000.bin" /
06-15-1998 00:00:00 "hotstart_06-15-1998_000000.bin" /
07-15-1998 00:00:00 "hotstart_07-15-1998_000000.bin" /
08-15-1998 00:00:00 "hotstart_08-15-1998_000000.bin" /
09-15-1998 00:00:00 "hotstart_09-15-1998_000000.bin" /
10-15-1998 00:00:00 "hotstart_10-15-1998_000000.bin" /
11-15-1998 00:00:00 "hotstart_11-15-1998_000000.bin" /
12-15-1998 00:00:00 "hotstart_12-15-1998_000000.bin" /
```

Figure 4.8. Example `transport_only.dat` file.

more model cells. This feature was originally designed to interface to groundwater contaminant transport model. The algorithm is described in Section 3.8.2.2 of the Theory Manual.

The bed source for an individual scalar is specified using the `BEDSOURCE` keyword in the `scalar_source.dat` file (Section 4.4). This keyword requires the names of two files.

The first file contains a list of files containing individual cumulative mass curve time series, an example of which is shown in Figure 4.9. Each record in this file contains a unique integer identifier and a file name. The file name specified contains a time series, in the format described in Section 4.10, that represents an individual source as a cumulative mass curve. An example is shown in Figure 4.10.

The second file is a list of "map" files. One map file is required for each computational mesh block. Each map file has a format similar to the computational mesh input file (Section 4.2). An example is shown in Figure 4.11. The first line of the map file contains two fields with the number of cells longitudinally (($i_{\max}$) and laterally ($j_{\max}$). The remainder of the file consists of one line per cell in the block, each line containing four fields:

1. longitudinal cell index (i)
2. lateral cell index (j)
3. integer identifier of the contaminant source time series that corresponds to an identifier in the source list file
4. fraction of the source time series allocated to this cell.

The cell indexes are not used by the model and are there only for the user's reference. The cells must be listed by longitudinal index (i) from upstream to downstream first then lateral index (j) from the right to left bank. The fractions should sum to 1.0 for each source time series, although the model does not check this.

A scalar bed source can have a water flux component. This flux indicates that a water source is carrying the scalar to the river bottom. The water flux is used by MASS2 only to "flush" the bed pore water and does not affect the hydrodynamic solution. The bed source water flux is specified using the `BEDFLOW` keyword in `scalar_source.dat`. As with `BEDSOURCE`, two file names are required that are formatted in the same manner as bed source files.

```
  651 "cfest/TMS-651-Tc99.DAT" /
10229 "cfest/TMS-10229-Tc99.DAT" /
10230 "cfest/TMS-10230-Tc99.DAT" /
10231 "cfest/TMS-10231-Tc99.DAT" /
10232 "cfest/TMS-10232-Tc99.DAT" /
10233 "cfest/TMS-10233-Tc99.DAT" /
```

Figure 4.9. Example bed source list file.

```
# cfest/TMS-10229-Tc99.DAT
07-01-1944 14:23:59     0.000000000000000E+00
12-31-1944 07:12:00     0.000000000000000E+00
07-01-1945 21:35:59     0.542246863297033E-17
12-31-1945 12:00:00     0.711723763822562E-13
07-02-1946 02:24:00     0.712335384706149E-13
12-31-1946 16:48:00     0.912544816985040E-13
07-02-1947 09:36:00     0.109436354373477E-12
01-01-1948 00:00:00     0.142336959236001E-12
07-01-1948 14:23:59     0.340892344872944E-11
12-31-1948 04:48:00     0.399680649635839E-11
07-01-1949 21:36:00     0.496363375262946E-11
12-31-1949 12:00:00     0.688563423106987E-11
07-02-1950 02:23:59     0.694715975377073E-11
12-31-1950 16:47:59     0.140848142674618E-10
07-02-1951 09:36:00     0.143354354963000E-10
01-01-1952 00:00:00     0.155261904573540E-10
07-01-1952 14:23:59     0.155317173137582E-10
12-31-1952 07:12:00     0.207801509149877E-10
07-01-1953 21:36:00     0.209028257114730E-10
12-31-1953 12:00:00     0.209362407102500E-10
07-02-1954 02:23:59     0.220765791467555E-10
12-31-1954 19:12:00     0.289004829869074E-10
07-02-1955 09:35:59     0.331946429554386E-10
01-01-1956 00:00:00     0.331946429554386E-10
07-01-1956 14:24:00     0.335044877976722E-10
12-31-1956 07:12:00     0.581729182069735E-10
07-01-1957 21:35:59     0.855828642866796E-10
12-31-1957 12:00:00     0.924427697601342E-10
07-02-1958 02:24:00     0.926687201837099E-10
12-31-1958 19:12:00     0.945465712686631E-10
07-02-1959 09:35:59     0.962226503189519E-10
```

Figure 4.10. Example bed source mass curve time series file.

```
"cfest/COV-001.DAT" /
"cfest/COV-002.DAT" /
"cfest/COV-003.DAT" /
"cfest/COV-004.DAT" /
"cfest/COV-005.DAT" /
"cfest/COV-006.DAT" /
"cfest/COV-007.DAT" /
"cfest/COV-008.DAT" /
"cfest/COV-009.DAT" /
"cfest/COV-010.DAT" /
```

Figure 4.11. Example bed source map list file. This example is for a 10-block domain.

4.10 Time Series Data Files

All time series data used in MASS2 for boundary conditions, meteorology, etc. are read from similarly formatted files. MASS2 reads the files and stores the time series in their entirety and linearly interpolates between times during the simulation.

4.10.1 Date/Time Format

MASS2 uses calendar dates for the input and output of simulation time. Where simulation time is required in any MASS2 input file, a consistent date/time format is used. The date and time are separated by white space. The date consists of the month, day, and year separated by a "–" character. The day and month may one or two digits; the year may have any number of digits. There is no assumption about century is made, so a year of 52 means the year 52 A.D. not 1952. The time consists of the hour, minute, and second separated by a ":" character The reading of dates and times is somewhat flexible. For example, the following are valid dates and times:

```
01-25-1974 10:45:25
1-6-25 9:18:03
12-6-13400 9:18:3.5
```

While MASS2 can read fractional seconds in the time, it does not write fractions of seconds in the output.

```
    3    5
    0    0   651   0.121199
    0    1   651   0.013468
    0    2     0   0.000000
    0    3     0   0.000000
    0    4     0   0.000000
    1    0   651   0.212236
    1    1   651   0.185684
    1    2   651   0.095724
    1    3   651   0.027079
    1    4   651   0.000156
    2    0 10229   1.000000
    2    1 10230   1.000000
    2    2 10231   1.000000
    2    3 10232   1.000000
    2    4 10233   1.000000
```

Figure 4.12. Example bed source map file. In this example, portions of scalar mass source 651 are assigned to seven cells. The other five sources (10229 through 10233) are assigned to individual cells.

4.10.2 Boundary Condition Data Files

MASS2 reads boundary conditions, source data, and other time series data from plain text files. The files are read using free-format Fortran 90. The first line of the file is ignored by MASS2, so it is usually used for a description of the file contents. Records in the remainder of the file are made up of several fields separated by white space and each record terminated with a "/." The first two fields of each record are the date and time in the format described in Section 4.10.1. The remainder of the record consists of one or more real values. An example boundary condition file is shown in Figure 4.13.

The number of values varies depending on what data is being supplied. For example, if a `TABLE` boundary condition with a `PART` qualifier is specified in `bcspecs.dat` (Section 4.3) one value will be expected for each cell index pair listed. Also, when an `ELEVEL` condition is specified, two values for each index pair are expected (stage and velocity, in that order).

```
# Snake River, Ice Harbor Dam: Spill (cfs)
03-31-1997 23:30:00       67600.000 /
04-01-1997 00:30:00       66800.000 /
04-01-1997 01:30:00       55300.000 /
04-01-1997 02:30:00       54700.000 /
04-01-1997 03:30:00       55600.000 /
04-01-1997 04:30:00       54700.000 /
04-01-1997 05:30:00       54700.000 /
04-01-1997 06:30:00       54700.000 /
04-01-1997 07:30:00       54700.000 /
04-01-1997 08:30:00       54700.000 /
04-01-1997 09:30:00       55700.000 /
04-01-1997 10:30:00       54800.000 /
04-01-1997 11:30:00       54800.000 /
04-01-1997 12:30:00       54800.000 /
04-01-1997 13:30:00       73700.000 /
04-01-1997 14:30:00       75800.000 /
04-01-1997 15:30:00       74500.000 /
04-01-1997 16:30:00       68800.000 /
04-01-1997 17:30:00       55100.000 /
04-01-1997 18:30:00       48600.000 /
04-01-1997 19:30:00       45200.000 /
04-01-1997 20:30:00       45100.000 /
04-01-1997 21:30:00       46000.000 /
04-01-1997 22:30:00       42500.000 /
```

Figure 4.13. Example of a boundary condition data file.

4.10.3 Meteorological Data File

Meteorological data is required when temperature or dissolved gas is simulated *and* surface heat exchange or air/water gas exchange is enabled in `scalar_source.dat` (Section 4.4). The

name of the file is specified in record 8 of the configuration file (Section 4.1). The flags to enable surface heat exchange and air/water gas exchange are also specified in that record.

The file is formatted as a boundary condition file (Section 4.10.2) with the fields listed in Table 4.5. An example meteorological data file is shown in Figure 4.14.

Table 4.5. Fields in the meteorology input file. Each record must contain all fields.

Field	Description	Units
1	date of the record, in the MASS2 format (e.g. 04-15-2002)	
2	time of the record, in the MASS2 format (e.g. 12:43:00)	
3	air temperature	°C
4	dew point temperature	°C
5	wind speed	m/sec
6	barometric pressure	mm Hg
7	net incoming short wave radiation	W/m^2

4.11 `initial_bed.dat`: Initial Bed File

The initial depth and composition of the bed can be specified with a set of files. If enabled using the flag in record 37 of the configuration file, a list of initial bed files, one for each block, is read from a file named `initial_bed.dat`. An example `initial_bed.dat` file is shown in Figure 4.15 for a 10 block domain. Each file to which this list refers has a format similar to the computational mesh input files (Section 4.2. The first line contains the range of *cell* indexes in the block (i.e., one less than the number of vertices specified in the computational mesh file for the block). The remainder of the file contains one line per cell, each having the following fields: cell longitudinal index (i), cell lateral index (j), the initial bed depth in cell (i, j), and the fraction of each transported sediment class initial in that cell. As with computational mesh files, the cell indexes are not used by MASS2 and are there to aid the user. An simple example of an initial bed data file is shown in Figure 4.16. This example is for a small block and only one transported sediment class.

4.12 Files for Spatially Varying Parameters

Several hydrodynamic and transport parameters (Table 4.6) are specified as constants in the configuration file (Section 4.1). Often it is useful to have these parameters vary over the domain.

Where the constant parameter is specified in the configuration file, the flag following the parameter value determines if the file containing the spatially values is read. For example, the default Manning's roughness coefficient is specified in record 25 of the configuration file. If the next field in that record is true (`T`), a file named `roughness_coeff.dat` is opened and read.

Each record specifies a new value and a logically rectangular region over which that value is applied.

```
#
04-02-1997 00:00:00     14.1    -1.9      5.1   765.4     0.0 /
04-02-1997 01:00:00     13.1    -1.9      5.1   765.5     0.0 /
04-02-1997 02:00:00     12.1    -2.9      4.1   765.6     0.0 /
04-02-1997 03:00:00      8.1    -0.9      2.6   765.8     0.0 /
04-02-1997 04:00:00      5.1     0.1      2.6   766.2     0.0 /
04-02-1997 05:00:00      4.1     0.1      2.6   766.4     0.0 /
04-02-1997 06:00:00      4.1     1.1      2.6   766.4     8.1 /
04-02-1997 07:00:00      4.1    -3.9      0.0   766.6   122.5 /
04-02-1997 08:00:00      4.1    -3.9      0.0   766.4   310.2 /
04-02-1997 09:00:00      4.1    -3.9      0.0   766.0   483.2 /
04-02-1997 10:00:00      4.1    -3.9      0.0   765.5   627.4 /
04-02-1997 11:00:00      4.1    -3.9      0.0   764.6   729.6 /
04-02-1997 12:00:00      4.1    -3.9      0.0   763.7   780.3 /
04-02-1997 13:00:00     -3.9    -3.9      0.0   763.0   775.0 /
04-02-1997 14:00:00     -3.9    -3.9      0.0   762.1   714.0 /
04-02-1997 15:00:00     -3.9    -3.9      0.0   761.3   603.0 /
04-02-1997 16:00:00     -3.9    -3.9      0.0   760.6   452.3 /
04-02-1997 17:00:00     -3.9    -3.9      0.0   759.8   275.4 /
04-02-1997 18:00:00     -3.9    -3.9      0.0   759.2    87.1 /
04-02-1997 19:00:00     -3.9    -3.9      0.0   758.6     0.0 /
04-02-1997 20:00:00     -3.9    -3.9      0.0   758.4     0.0 /
04-02-1997 21:00:00     -3.9    -3.9      0.0   757.7     0.0 /
04-02-1997 22:00:00     -3.9    -3.9      0.0   756.7     0.0 /
04-02-1997 23:00:00     -3.9    -3.9      0.0   756.2     0.0 /
```

Figure 4.14. Example meteorology data file.

```
"bed/coarse-depth.001"  /
"bed/coarse-depth.002"  /
"bed/coarse-depth.003"  /
"bed/coarse-depth.004"  /
"bed/coarse-depth.005"  /
"bed/coarse-depth.006"  /
"bed/coarse-depth.007"  /
"bed/coarse-depth.008"  /
"bed/coarse-depth.009"  /
"bed/coarse-depth.010"  /
```

Figure 4.15. Example initial_bed.dat file.

```
    5     6
    1     1        1.000        1.000 /
    1     2        1.000        1.000 /
    1     3        1.000        1.000 /
    1     4        1.000        1.000 /
    1     5        1.000        1.000 /
    1     6        1.000        1.000 /
    2     2        2.000        1.000 /
    2     2        1.000        1.000 /
    2     3        1.000        1.000 /
    2     4        1.000        1.000 /
    2     5        1.000        1.000 /
    2     1        1.000        1.000 /
    3     2        2.000        1.000 /
    3     2        1.000        1.000 /
    3     3        1.000        1.000 /
    3     4        1.000        1.000 /
    3     5        1.000        1.000 /
    3     6        1.000        1.000 /
    4     1        2.000        1.000 /
    4     2        1.000        1.000 /
    4     3        1.000        1.000 /
    4     4        1.000        1.000 /
    4     5        1.000        1.000 /
    4     6        1.000        1.000 /
    5     1        2.000        1.000 /
    5     2        1.000        1.000 /
    5     3        1.000        1.000 /
    5     4        1.000        1.000 /
    5     5        1.000        1.000 /
    5     6        1.000        1.000 /
```

Figure 4.16. Example initial bed data file.

1. block number
2. parameter value
3. starting longitudinal index ($i_{\min}$)
4. ending longitudinal index ($i_{\max}$)
5. starting lateral index ($j_{\min}$)
6. ending lateral index ($j_{\max}$).

An example `roughness_coeff.dat` file is shown in Figure 4.17. In this example, the domain was divided into three parts. Blocks 4 and 10 were split (lines 4-5, and 11-12) in this

division. A different value of Manning's roughness coefficient was used for each of the three areas. In this case, values for all of the domain were specified, but this was not necesary. Any part of the domain not specified in the `roughness_coeff.dat` would have been assigned the default value from the configuration file.

Table 4.6. Files used to specify spatially varying parameters. The configuration file record shown specifies the default, spatially constant value and whether the spatially varying values are read.

Input File Name	Parameter	Configuration File Record
`roughness_coeff.dat`	bed roughness coefficient, Chezy C or Manning's n	25
`eddy_coeff.dat`	eddy diffusivity, ft^2/sec	22
`kx_coeff.dat`	longitudinal diffusivity for all transported scalars, ft^2/sec	24
`ky_coeff.dat`	lateral diffusivity for all transported scalars, ft^2/sec	24

```
1  0.0266    1 267  1 89
2  0.0266    1  90  1 50
3  0.0266    1 114  1 40
4  0.0266    1 125  1 89
4  0.0278  126 159  1 89
5  0.0278    1  85  1 50
6  0.0278    1 299  1 40
7  0.0278    1 160  1 21
8  0.0278    1  90  1 30
9  0.0278    1 133  1 69
10 0.0278    1 123  1 89
10 0.0259  124 278  1 89
11 0.0259    1 121  1 89
12 0.0259    1 110  1 72
13 0.0259    1 741  1 89
14 0.0259    1 304  1 78
15 0.0259    1 250  1 12
16 0.0259    1 157  1 89
```

Figure 4.17. Example `roughness_coeff.dat` file showing regions where Manning's roughness coefficient differ from the default.

4.13 Total Dissolved Gas Air-Water Exchange Coefficients File

When total dissolved gas is simulated, gas exchange with the atmosphere can be enabled using the the `AIREXCH` keyword `scalar_source.dat` (Section 4.4). In this case, the file specified with the `PARAMETERS` keyword will be read and is expected to contain a single record with up to

four real coefficients to the gas exchange formula (equation 2.23, Theory Manual). The coefficients are read in the following order: a, b, c, d. An example file is shown in Figure 4.18.

```
0.6885 -0.5025 0.1535 -0.0045 / a, b, c, d
```

Figure 4.18. Example total dissolved gas air-water exchange coefficients file.

4.14 `hotstart.bin`: Hot Start

Initial conditions can be read from the results of a previous simulation saved in a hot-start file (Section 5.6). If enabled in record 12 of the configuration file, MASS2 will read a hot start file named `hotstart.bin`. This file contains all necessary information about the previous simulation so that it may be continued from when the hot-start file was written.

When a hot-start file is read by MASS2, it uses whatever part of the previous state that it can. For example, in transport mode, scalar transport simulation will be initialized from the hot-start only if it exists. This allows the use of a hot-start from a hydrodynamics mode simulation to be used to start a transport mode simulation.

5.0 Output Files

5.1 Simulation Log Files

In all simulation modes, MASS2 creates three plain text files named `error_warning.out`, `status.out`, and `output.out`. The `error_warning.out` file is used to record serious errors that occur during the simulation. This includes errors or warnings about input files and their contents and negative depths. If wetting and drying are not enabled, a negative depth causes the simulation to be aborted. Otherwise, the depth is set to the zero depth. MASS2 will report the time and cell location of the negative depth to aid in resolving the problem. All messages written to `error_warning.out` are also written to standard output (the screen) during the simulation. This output file helps to record problems if the screen output is lost.

The `status.out` file is used by MASS2 to record activity as the simulation proceeds. The primary activities recorded are memory allocation and opening and closing of files. This is sometimes helpful in identifying the reason for a simulation crash.

MASS2 also creates a file named `output.out`. This file is used for debugging the model and has little use for the average user.

5.2 `gridplot1.dat`: Grid Output

The output file `gridplot1.dat` is a rendering of the computational mesh read by MASS2. It is used to verify that computational mesh was assembled and read correctly and to help with the specification of boundary conditions (Section 4.3) and gage output locations (Section 4.6). It can also be used to visualize the bathymetry represented by the computational mesh. The file is always written, regardless of simulation mode.

The file is formatted so that it can be read directly by Tecplot as an ASCII data file. One zone is created for each grid block. The data variables are the grid vertex coordinates (`x` and `y`) and the elevation at the vertex (`zbot`). If the debug mode is enabled, using the flag on record 9 of the configuration file (Section 4.1), the grid written to `gridplot1.dat` will also contain the ghost cells (see Section 3.1 of the Theory Manual for discussion of ghost cells). This will cause the cell indexing used in Tecplot to be offset. This is intended only for verification of ghost cell generation for block connections.

5.3 `mass_source_monitor.out`: Block Mass Source Output

The MASS2 hydrodynamic solution algorithm attempts to minimize the mass source error of the domain (see Theory Manual, Section 3.3.1). The mass source error can be described as the fluid flux imbalance for the entire block. Understanding how the mass source error changes during

a simulation can be very helpful to diagnose problems or to ensure hydrodynamic convergence (as described in Section 3.3, for example).

If gage output is enabled in record 13 of the configuration file, block mass source is output for hydrodynamics simulations. A text file named `mass_source_monitor.out` is created in the current directory during the simulation. The file is plain text with the following fields separated by white space:

1. simulation date
2. simulation time
3. number of hydrodynamic (outer) iterations performed during the previous time step
4. mass source error, in cfs, for each block in the domain.

An example `mass_source_monitor.out` file is shown in Figure 5.1.

Each line in `mass_source_monitor.out` is limited to 20 blocks. It would be more convenient to have all blocks on a single line. The limitation was necessary because some Fortran 90 compilers limit the length of an output line. With 20 blocks per line, the format `mass_source_monitor.out` is consistent across all of the compilers used.

```
# mass source history - summation of the mass source in each block
#      total mass imbalance for each block in ft3/sec
#date        time                  1            2            3
04-01-1996  00:05:00      13    482.5        1963.        45.37
04-01-1996  00:10:00      13    1007.        1872.        64.75
04-01-1996  00:15:00      13    174.3        567.3        35.30
04-01-1996  00:20:00      13    25.74        159.8        9.103
04-01-1996  00:25:00       9    3.480        8.324       0.6350
04-01-1996  00:30:00      13    9.853        29.01        1.442
04-01-1996  00:35:00      13    6.507        36.40        1.903
04-01-1996  00:40:00      13    4.857        30.79        1.682
04-01-1996  00:45:00      13    3.555        20.59        1.067
04-01-1996  00:50:00      13    2.390        13.04       0.6443
04-01-1996  00:55:00      12    1.480        8.294       0.4054
04-01-1996  01:00:00       6    9.405        8.583        1.109
04-01-1996  01:05:00       5    8.256        8.365        1.245
04-01-1996  01:10:00       3    8.859        10.00        1.857
04-01-1996  01:15:00       2    8.001        9.376        1.722
```

Figure 5.1. Example `mass_source_monitor.out` for a simulation with three computational mesh blocks.

5.4 Two-Dimensional Output

MASS2 can save the state of the entire current simulated domain at regular intervals by enabling NetCDF output in record 39 and/or CGNS output in record 40 of the configuration file. Two-dimensional output is saved at regular intervals. The interval is specified in record 38 of the configuration file. The initial conditions and final state of the simulation are always saved in any two-dimensional output.

5.4.1 Diagnostic Hydrodynamic Variables

Diagnostic hydrodynamic variables can be saved with the two-dimensional output.

- longitudinal and lateral velocity components in computational space,
- velocity magnitude
- water surface elevation
- bed shear
- Courant number
- Froude number.

These values can all be calculated from hydrodynamic state variables and are often useful or even necessary. However, saving the diagnostic variables can use a large amount of disk space. So, output of these variables is optional and enabled by a flag in record 39 of the configuration file.

5.4.2 Output Averaging

Output averaging is controlled by the flag with the two-dimensional output frequency in record 38 of the configuration file. Normally the flag is set to false. In that case, two-dimensional output, in either format, is the instantaneous state simulated at the output time. It is sometimes useful to have an average value for the output period.

5.4.3 NetCDF Format

The NetCDF file format (Rew et al. 1997) was originally developed to store data related to atmospheric models. The format is designed to store a single (logically) rectangular domain of many dimensions. NetCDF data is stored in a binary format that is independent of computer architecture. For example, a NetCDF file produced on a Windows PC can be read and manipulated on a Silicon Graphics workstation (and vice versa), even though those two platforms use different binary representations of integers and floating point numbers.

The flag in record 39 of the configuration file is used to enable two-dimensional NetCDF output. When enabled, simulation results are written to a file named `plot.nc` in the current directory.

Simulated values are output at cell centers. Values along block edges are pre-interpolated. The locations of output data for an example block are shown in Figure 5.2. Table 5.1 lists the variables written to the NetCDF file during a MASS2 simulation.

The NetCDF format and library software are mature and have been in widespread use for several years. Consequently, there are several software tools available for manipulating NetCDF files. The most useful one is the NetCDF operators suite (NCO Zender 2004).

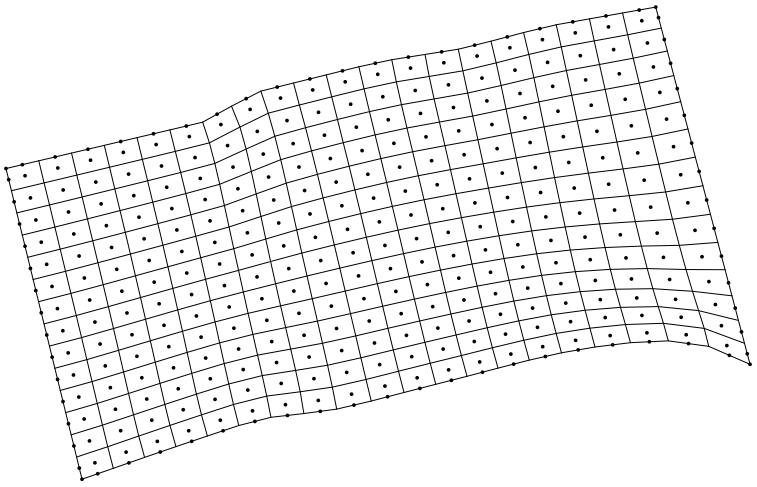


Figure 5.2. Output locations for two-dimensional NetCDF output for an example computational mesh. The mesh is shown as lines and the output locations as block dots. Block edge values are copied from the adjacent cell or averaged with the value neighboring block.

Table 5.1. Data variable names used in two-dimensional NetCDF output.

Name	Dimensions	Description	Units
Dimension Variables			
`block`		Number of mesh blocks	
`eta`		Largest number of longitudinal (upstream to downstream) output locations	
`xi`		Largest number of lateral (right to left bank) output locations	
`time`		Number of time steps (unlimited)	
`tslen`		Length of `timestamp` string (20)	
Mesh Variables			

Table 5.1. Data variable names used in two-dimensional NetCDF output (continued).

Name	Dimensions	Description	Units
`etamax`	(`block`)	Number of longitudinal output locations in each block	
`ximax`	(`block`)	Number of lateral output locations in each block	
`x`	(`xi`, `eta`, `block`)	Cartesian x-coordinate (easting) of each output location	ft
`y`	(`xi`, `eta`, `block`)	Cartesian y-coordinate (northing) of each output location	ft
`zbot`	(`xi`, `eta`, `block`)	River bottom elevation	ft
`hp1`	(`xi`, `eta`, `block`)	Computational mesh metric	ft
`hp2`	(`xi`, `eta`, `block`)	Computational mesh metric	ft
`gp12`	(`xi`, `eta`, `block`)	Computational mesh metric	ft
Hydrodynamic Variables			
`ucart`	(`time`, `xi`, `eta`, `block`)	Cartesian velocity in the x direction (eastward)	ft/sec
`vcart`	(`time`, `xi`, `eta`, `block`)	Cartesian velocity in the y direction (northward)	ft/sec
`depth`	(`time`, `xi`, `eta`, `block`)	Flow depth	ft
`isdry`[(a)]	(`time`, `xi`, `eta`, `block`)	Flag (1.0 = true) indicating the cell is dry.	
`isdead`[(b)]	(`time`, `xi`, `eta`, `block`)	Flag (1.0 = true) indicating the cell is specified as dead in the `bcspecs.dat` file.	
Diagnostic Hydrodynamic Variables			
`uvel`	(`time`, `xi`, `eta`, `block`)	Longitudinal velocity (U in computational coordinates)	ft/sec
`vvel`	(`time`, `xi`, `eta`, `block`)	Lateral velocity (V in computational coordinates)	ft/sec
`vmag`	(`time`, `xi`, `eta`, `block`)	Velocity magnitude $\left(\sqrt{U^2+V^2}\right)$	ft/sec

(a) Included only when wetting and drying is enabled.
(b) Included only when dead zones are specified in `bcspecs.dat` (Section 4.3.3).

Table 5.1. Data variable names used in two-dimensional NetCDF output (continued).

Name	Dimensions	Description	Units
wsel	(time, xi, eta, block)	Water surface elevation (depth + wsel)	ft
shear	(time, xi, eta, block)	Bed shear stress	lbf/ft^2
courant	(time, xi, eta, block)	Cell Courant number	
froude	(time, xi, eta, block)	Cell Froude number	
Predefined Water Quality Variables			
tdgconc	(time, xi, eta, block)	Total dissolved gas (TDG) concentration	mg/L
tdgpress	(time, xi, eta, block)	TDG partial pressure	mm Hg
tdgdeltap	(time, xi, eta, block)	TDG partial pressure above saturation pressure	mm Hg
tdgsat	(time, xi, eta, block)	Ratio of TDG partial pressure to saturation TDG partial pressure	percent
temperature	(time, xi, eta, block)	Water temperature	°C
User-defined Scalar Quantity Variables			
species(c)	(time, xi, eta, block)	Concentration of scalar in water column	(d)
part(e)	(time, xi, eta, block)	Concentration of particulate species in water column	(f)
fract(g)	(time, xi, eta, block)	Concentration of sediment fraction in water column	(h)
Bed Variables			
beddepth	(time, xi, eta, block)	Bed depth	ft
fract-depos	(time, xi, eta, block)	Deposition rate of sediment fraction *fract*	*mass*(i)/ft^2/sec
fract-erode	(time, xi, eta, block)	Erosion rate of sediment fraction *fract*	*mass*/ft^2/sec
fract-bed	(time, xi, eta, block)	Mass of sediment fraction *fract* in the bed	*mass*/ft^2

(c) User defined generic dissolved scalar species name.
(d) User-defined concentration units.
(e) User defined particulate scalar species name.
(f) User-defined concentration units.
(g) User defined sediment fraction name.
(h) User-defined concentration units.
(i) User defined mass units (usually kg).

Table 5.1. Data variable names used in two-dimensional NetCDF output (continued).

Name	Dimensions	Description	Units
fract-bedmass	(time, xi, eta, block)	Mass of sediment fraction *fract* within the bed cell	*mass*
species-pore	(time, xi, eta, block)	Bed pore water concentration of scalar *species*	*mass*/m^2
species-bed	(time, xi, eta, block)	Mass of scalar species in the bed	*mass*/m^2
species-bedmass	(time, xi, eta, block)	Mass of scalar species in the bed	*mass*/cell
part-depos	(time, xi, eta, block)	Deposition rate of particulate scalar part in the bed	*mass*/ft^2/sec
part-erode	(time, xi, eta, block)	Erosion rate of particulate scalar part in the bed	*mass*/ft^2/sec
part-bed	(time, xi, eta, block)	Mass of particulate scalar part in the bed	*mass*/ft^2
part-bedmass	(time, xi, eta, block)	Mass of particulate scalar part in the bed	*mass*/cell

5.4.4 CGNS Format

Two-dimensional simulation results can be written to files using the Computational Fluid Dynamics (CFD) General Notation System (CGNS) (Rumsey et al. 2002; CGNS Project Group 2003). This format is newer than NetCDF and has only recently been used in MASS2. Consequently, the CGNS format is not as mature as NetCDF, but it is gaining acceptance.

In general, CGNS output is functionally the same as NetCDF. In multi-block cases, CGNS uses much less disk space than NetCDF. Because NetCDF was designed for rectangular domains only, MASS2 NetCDF files can take too much storage for applications with widely varying block sizes. When blocks of different sizes are used, a large portion of the resulting output file is unused, because space is allocated in the NetCDF file based on the largest block dimensions in the domain.

Record 40 of the configuration file is used to control CGNS output. When CGNS output is enabled in the configuration file, a file named grid.cgns is used to store computational mesh coordinates and metric coefficients. Simulation results are stored in a series of numbered files named plot000.cgns, plot001.cgns, etc. Each plot*.cgns file is used to store a specified number of output times and is linked to the grid.cgns file for computational mesh coordinates. This is helpful when the size of single files become larger than the computer's operating system allows. Because of the links between them, the plot*.cgns must be kept with the grid.cgns file whenever they are used.

5.5 gage.nc: Gage Output

If gage output is enabled in record 13 of the configuration file, MASS2 attempts to read a list of gage locations from gage_control.dat (Section 4.6). If any locations are read, a file called gage.nc is created during the simulation. This file uses NetCDF (Rew et al. 1997); its structure is shown in Figure 5.3. The state of the specified cells is written to this file at the interval specified in record 41 of the configuration file. Time series can be extracted from gage.nc using the Perl script mass2gage.pl (Section 6.2.1), as shown in Figure 5.4.

The variables written to the gage output are a subset of those written to NetCDF two-dimensional output (Table 5.1). The gage output does not contain the mesh metric or the diagnostic variables.

5.6 Hot Start Files

When enabled, MASS2 will save the complete state of the simulation at regular intervals specified in record 11 of the configuration file. This state includes all necessary information about the current hydrodynamic and transport solutions to allow the simulation to be restarted at that time. Each hot-start file is named uniquely according to the simulation time at which it was written. For example, a hot-start file written at April 3, 2000, 6:00 am is named

```
hotstart_04-03-2000_060000.bin.
```

This file is actually written as plain text so it is portable and the same hot-start file is portable, i.e., it can be used on a different computer platform than the one that produced it. However, the format of the file is not meant to be readable by humans.

Writing hot-start files during a MASS2 simulation not only allows the user to restart the simulation with different parameters or in a different mode but also provides some insurance against simulation and system crashes. If the model or computer system crashes, at least part of the simulation is saved and can be continued from the hot start file. Writing hot-start files is also necessary for preparing hydrodynamic conditions for transport-only mode simulations.

```
netcdf gage {
dimensions:
        gage = 3 ;
        time = UNLIMITED ; // (61 currently)
        tslen = 20 ;
        idlen = 40 ;
variables:
        int block(gage) ;
        int eta(gage) ;
        int xi(gage) ;
        char gage_name(gage, idlen) ;
        double time(time) ;
                time:Units = "days since 1900-01-01 00:00:00" ;
        float elapsed(time) ;
                elapsed:Units = "hours" ;
                elapsed:Description = "Elapsed Simulation Time" ;
        char timestamp(time, tslen) ;
        float wsel(time, gage) ;
                wsel:Units = "feet" ;
                wsel:Description = "Water Surface Elevation" ;
                wsel:units = "feet" ;
                wsel:long_name = "Water Surface Elevation" ;
                wsel:_FillValue = 9.96921e+36f ;
        float depth(time, gage) ;
                depth:Units = "feet" ;
                depth:Description = "Depth" ;
                depth:units = "feet" ;
                depth:long_name = "Depth" ;
                depth:_FillValue = 9.96921e+36f ;
        float vmag(time, gage) ;
                vmag:Units = "feet/second" ;
                vmag:Description = "Velocity Magnitude" ;
                vmag:units = "feet/second" ;
                vmag:long_name = "Velocity Magnitude" ;
                vmag:_FillValue = 9.96921e+36f ;
        float uvel(time, gage) ;
                uvel:Units = "feet/second" ;
                uvel:Description = "Longitudinal Velocity" ;
                uvel:units = "feet/second" ;
                uvel:long_name = "Longitudinal Velocity" ;
                uvel:_FillValue = 9.96921e+36f ;
        float vvel(time, gage) ;
                vvel:Units = "feet/second" ;
                vvel:Description = "Lateral Velocity" ;
                vvel:units = "feet/second" ;
                vvel:long_name = "Lateral Velocity" ;
                vvel:_FillValue = 9.96921e+36f ;
        float isdry(time, gage) ;
                isdry:Units = "none" ;
                isdry:Description = "Dry Cell Flag" ;
                isdry:units = "none" ;
                isdry:long_name = "Dry Cell Flag" ;
                isdry:_FillValue = 9.96921e+36f ;
}
```

Figure 5.3. Structure of an example NetCDF gage output file, `gage.nc`. This listing was produced with the NetCDF utility `ncdump`.

```
> perl mass2gage.pl -l gage.nc
MASS2 Gage Output File:
         "gage.nc"
1 time slices:
        starting: 03-19-1999 12:00:00
          ending: 03-19-1999 12:00:00

Available Gage Locations
-----------------------------------------------------
Gage Name                            Block   Eta    Xi
-----------------------------------------------------
   1 T54LBC piezometer                   1   167    83
   2 T61IRC piezometer                   2    63    27
   3 T64RBC piezometer                   4   117     9
   4 T81RBC piezometer                  12    38    47
   5 T90RBC piezometer                  13   228    51
   6 T94RBC piezometer                  13   451    15
   7 T101LBC piezometer                 14    24    63
   8 downstream extent                  16   155    40
   9 ERC 100-D                           1    22     7
  10 ERC 100-H                           4   115     9
  11 ERC 100-F                          10   116     9
  12 ERC 100-D Alternate                 1    22    10
  13 trouble spot                       11     4    16
  14 trouble spot upstream              11     3    16
  15 trouble spot downstream            11     5    16
  16 trouble spot west                  11     4    15
  17 trouble spot east                  11     4    17
-----------------------------------------------------

Available Time-Dependant Variables:
  8 wsel                 Water Surface Elevation, feet
  9 depth                Depth, feet
 10 vmag                 Velocity Magnitude, feet/second
 11 uvel                 Longitudinal Velocity, feet/second
 12 vvel                 Lateral Velocity, feet/second
 13 isdry                Dry Cell Flag, none
> perl mass2gage.pl -v depth -g 8 gage.nc
03-19-1999 12:00:00           8.369
03-19-1999 13:00:00          9.9153
03-19-1999 14:00:00          9.8377
03-19-1999 15:00:00          9.7396
03-19-1999 16:00:00          9.6508
03-19-1999 17:00:00           9.562
03-19-1999 18:00:00          9.4928
```

Figure 5.4. Example of using the `mass2gage.pl` script to extract time series data from `gage.nc` output. The first use of the script (in bold) produces a listing of the gage locations and the available variables. The second use obtains the flow depth time series for gage 8.

6.0 Utility Reference

Several utility programs have been developed to aid in the application of MASS2. This chapter briefly documents the utilities that are used most often.

6.1 `cartgrid` Utility

The `cartgrid` utility is a stand-alone Fortran 90 program for generating Cartesian computational meshes for use with MASS2. The program is interactive (Figure 6.1), prompting the user for the information needed to construct a rectangular mesh:

- longitudinal (upstream/downstream) cell spacing
- lateral (left/right bank) cell spacing
- number of longitudinal cell vertices (downstream nodes)
- number of lateral cell vertices (cross stream bank nodes)
- coordinates of the block origin (x, y)
- upstream to downstream bottom slope
- downstream bottom elevation.

Given the above information, `cartgrid` produces a computational mesh file named `grid.out` that can be used with MASS2. The mesh describes a bed uniformly sloping from upstream to downstream.

6.2 Perl scripts

Two utility programs have been developed to post-process MASS2 output. These programs were written in an interpreted language called Perl.[(a)] The Perl interpreter is freely available and comes with most Linux distributions. Windows distributions are also available, but the MASS2 scripts documented in this section have not been tested on Windows.

Descriptions of the programs are given below. To use them, a Perl interpreter must be available. The utilities require Perl version 5.6 or later along with Perl Data Language (PDL) module (version 2.2 or later) and the PDL::NetCDF module (version 0.86).

(a) See `http://www.perl.org`.

```
> cartgrid
 This program create rectangular grids.
 No checks are made on data input so think before you type!
 Input longitudinal spacing (delta x) desired
0.0455
 Input lateral spacing (delta y) desired
0.0455
 Input number of downstream nodes desired
161
 Input number of cross stream nodes desired
41
 Input downstream starting x coordinate
-1.820
 Input starting y coordinate
0
 Enter name of bottom elevation file (RETURN for none)
<enter>
 Input slope
0
 Input downstream bottom elevation
0
 Thanks! Output file is grid.out
>
```

Figure 6.1. Sample `cartgrid` session. This session was used to produce the mesh in validation test presented in Section 4.1.9 of the Theory Manual. The mesh was produced in metric units first than converted to English.

Documentation for some utility scripts follows. The documentation was generated using the Perl utility `pod2latex`. The documentation shown below can be seen by running `perldoc` on the script file. See the Perl documentation for more information.

6.2.1 mass2gage.pl

Extract data from a MASS2 gage output file (NetCDF format).

SYNOPSIS

perl **mass2gage.pl -l** *file*

perl **mass2gage.pl -v** *var* **-g** *gage* [**-C**|**-M**] [**-1**] [**-D**] **-X** *n*] [**-o** *output*] *file*

DESCRIPTION

This script is used to extract data for one variable and gage from a MASS2 gage output file. It is primarily intended to be used to check a simulation while in progress.

OPTIONS

-l

List the gages and time-dependant variables in *file* and exit.

-v *var*

(required) Extract the *var* time-dependant variable from *file*; *var* may be either an integer or a variable name (as long as the name does not start with a number), either of which can be obtained using **-l**.

-g *gage*

Extract data from the *gage* location; *gage* may be either an integer or a gage location name (as long as the name does not start with a number), either of which can be obtained using **-l**.

-C

Output a cumulative frequency distribution; normally, a time series is output, this option will cause the data from the specified gage to be sorted and assigned an exceedance probability.

-D

If the *file* contains the variable `isdry`, extract records for *var* only when `isdry` is zero; applies only to the extraction of a time series; a CFD extraction will still contain all values.

-o *output*

Send extracted data to *output* (does not work with **-l**).

-1

Add a line at the top of the output (line 1) containing some information about the extracted data.

-M

Format as a MASS1/MASS2 boundary condition file (implies -1).

-X *n*

Skip the first *n* time records in the gage file, to avoid a warm up period, for example.

EXAMPLES

This is the output from a listing (**-l**) of a particular gage.nc file:

```
> \textbf{perl mass2gage.pl -l gage.nc }
MASS2 Gage Output File:
         "gage.nc"
1 time slices:
        starting: 03-19-1999 12:00:00
          ending: 03-19-1999 12:00:00


Available Gage Locations
-----------------------------------------------------
Gage Name                              Block   Eta    Xi
-----------------------------------------------------
   1 T54LBC piezometer                     1   167    83
   2 T61IRC piezometer                     2    63    27
   3 T64RBC piezometer                     4   117     9
   4 T81RBC piezometer                    12    38    47
   5 T90RBC piezometer                    13   228    51
   6 T94RBC piezometer                    13   451    15
   7 T101LBC piezometer                   14    24    63
   8 downstream extent                    16   155    40
   9 ERC 100-D                             1    22     7
  10 ERC 100-H                             4   115     9
  11 ERC 100-F                            10   116     9
  12 ERC 100-D Alternate                   1    22    10
  13 trouble spot                         11     4    16
  14 trouble spot upstream                11     3    16
  15 trouble spot downstream              11     5    16
  16 trouble spot west                    11     4    15
  17 trouble spot east                    11     4    17
-----------------------------------------------------


Available Time-Dependent Variables:
  8 wsel                 Water Surface Elevation, feet
  9 depth                Depth, feet
```

```
 10 vmag                 Velocity Magnitude, feet/second
 11 uvel                 Longitudinal Velocity, feet/second
 12 vvel                 Lateral Velocity, feet/second
 13 isdry                Dry Cell Flag, none
```

Depth data is extracted from the same file:

```
03-19-1999 12:00:00          8.369
03-19-1999 13:00:00         9.9153
03-19-1999 14:00:00         9.8377
03-19-1999 15:00:00         9.7396
03-19-1999 16:00:00         9.6508
03-19-1999 17:00:00          9.562
03-19-1999 18:00:00         9.4928
```

6.2.2 mass2slice.pl

Extract profile and cross section data from MASS2 plot output files.

SYNOPSIS

perl **mass2slice.pl** [**-d**] [-a] [**-i**|**-j**] [**-t** *indices*|**-l**] [**-o** *output*] *file variable block index* [*block index ...*]

perl **mass2slice.pl -p** [**-t** *indices*|**-l**] [**-o** *output*] *file variable block i j*

DESCRIPTION

mass2slice.pl is used to extract slices of data from the NetCDF format MASS2 plot output file. Slices can be made either longitudinally (**-i**) or laterally (**-j**) across multiple blocks. By default, all times are output separated by a blank line (useful for plotting in gnuplot).

OPTIONS

-a

Average the variable across the profile or cross section to produce one value.

-d

Place the date/time in the first two columns of the output.

-D

For **-i** and **-j** slices, do not output any points where the cell is dry. This option is ignored if there is no wet/drying information in *file*.

-i

Extract a profile. Distance is computed from upstream to downstream. The *index* is the lateral index.

-j

Extract a cross section. Distance is computed from the right to left bank (looking downstream). The *index* is the longitudinal index.

-p

Output a timeseries at a single point rather than a slice. If this option is used, both the *i* and *j* indices of the point (cell actually) are expected to be on the command line.

-t *index*

Select a specific time, specified by *index*, to extract. By default all times are extracted, and their time stamp is placed in the output.

-l

Extract only the last time in the plot output file. The **-t** is ignored if this option is specified.

-o *output*

Send data to *output* instead of standard output.

EXAMPLES

This script is typically used to provide data for profile plotting. The following gnuplot script will plot a water surface elevation profile from a three block domain:

```
plot '<perl mass2slice.pl -t 1 -i plot.nc wsel 1 5 2 10 3 5' \
       using 3:4 with l 1, \
     '<perl mass2slice.pl -l -i plot.nc wsel 1 5 2 10 3 5' \
       using 3:4 with l 3, \
     '<perl mass2slice.pl -i plot.nc zbot 1 5 2 10 3 5' \
       using 3:4 with l 7
```

Block 2 is either aligned differently or of a different resolution. The resulting plot will show three curves: the initial conditions (`-t 1, wsel`), the final conditions (`-l, wsel`), and the bottom elevation (`zbot`).

SEE ALSO

gnuplot(1)

7.0 References

CGNS Project Group. 2003. *CFD General Notation System, Overview and Entry-Level Document*. Version 2.0.7, Available URL: http://www.grc.nasa.gov/WWW/cgns/overview/index.html.

Kincaid CT, RW Bryce, PW Eslinger, CAB J. M. Becker, AL Bunn, CR Cole, EJ Freeman, GR Guensch, DG Horton, GV Last, TB Miley, WA Perkins, WE Nichols, M Oostrom, MC Richmond, DL Strenge, and PD Thorne. 2001. "Development of a Site-Wide System Assessment Capability." Presented at the Waste Management 2001 Symposium, February 25 - March 1, 2001, sponsored by the University of Arizona, Tuscon, Arizona.

McMichael GA, WA Perkins, CJ McMurray, YJ Chien, CL Rakowski, A Coleman, MC Richmond, J Vucelick, EV Arntzen, RP Mueller, CA Duberstein, and J Lukas. 2003. *Subyearling Chinook Salmon Stranding in the Hanford Reach of the Columbia River*. PNWD-3308, Battelle-Pacific Northwest Division, P.O. Box 999, Richland, Washington 99352. Prepared for Grant County Public Utility District No. 2.

Patankar S. 1980. *Numerical Heat Transfer and Fluid Flow.* Hemisphere, New York, New York.

Perkins W, M Richmond, and G McMichael. 2004. "Two-Dimensional Modeling of Time-Varying Hydrodynamics and Juvenile Chinook Salmon Habitat in the Hanford Reach of the Columbia River." In *Proceedings of the World Water and Environmental Resources Congress*. ASCE. Presented at conference held June 27-July 1 in Salt Lake City.

Perkins WA and MC Richmond. 2004. *MASS2, Modular Aquatic Simulation System in Two Dimensions, Theory and Numerical Methods*. PNNL-14820-1, Pacific Northwest National Laboratory, Richland, Washington 99352.

Rew R, G Davis, S Emmerson, and H Davies. 1997. *NetCDF Users Guide for FORTRAN, An Access Interface for Self-Describing, Portable Data*. University Center for Atmospheric Research, Unidata Program Center, P.O. Box 3000, Boulder, Colorado 80307. Available URL: `http://www.unidata.ucar.edu/packages/netcdf/fguide.pdf`.

Richmond M, W Perkins, and Y Chien. 2000. *Numerical Model Analysis of System-wide Dissolved Gas Abatement Alternatives*. PNWD-3245, Battelle Pacific Northwest Division, P.O. Box 999, Richland, Washington, 99352. Prepared for the U.S. Army Corps of Engineers, Walla Walla District under Contract DACW68-96-D-0002.

Richmond M, W Perkins, and T Scheibe. 1999. *Two-Dimensional Hydrodynamic, Water Quality, and Fish Exposure Modeling of the Columbia and Snake Rivers. Part 1: Summary and Model Formulation.* Final Report, Battelle Pacific Northwest Division, P. O. Box 999, Richland, Washington, 99352. Prepared for the U.S. Army Corps of Engineers, Walla Walla District under Contract DACW68-96-D-0002.

Rumsey CL, DMA Poirier, RH Bush, and CE Towne. 2002. *CFD General Notation System, A User's Guide To CGNS*. CGNS Project Group. Version 1.1.4, Available URL: `http://www.grc.nasa.gov/WWW/cgns/user/index.html`.

Spasojevic M and F Holly, Jr. 1990. "2-D Bed Evolution in Natural Watercourses New Simulation Approach." *Journal of Waterway, Port, Coastal, and Ocean Engineering* 116(4):425–443.

Steinbrenner J, N Wyman, and J Chawner. 2000a. "Development and Implementation of Gridgen's Hyperbolic PDE and Extrusion Methods." presented at the AIAA 38th Aerospace Sciences Meeting, 10-13 Jan 2000, Reno, NV. AIAA paper no. 2000-0679.

Steinbrenner J, N Wyman, and J Chawner. 2000b. "Fast Surface Meshing on Imperfect CAD Models." In *Proceedings of the 9th International Meshing Roundtable, 02-05 October 2000, New Orleans, SANDIA Report SAND2000-2207*, pp. 33–41.

Zender C. 2004. *NCO User's Guide*. Department of Earth System Science, University of California, Irvine, California. Available URL: `http://nco.sourceforge.net/\#RTFM`.

Zhou JG. 1995. "Velocity-Depth Coupling in Shallow-Water Flows." *Journal of Hydraulic Engineering* 121(10):717–724.

Appendix A

Input Files from Validation Applications

Appendix A – Input Files from Validation Applications

In this appendix, input files for the Modular Aquatic Simulation System in Two Dimensions (MASS2) are presented from some of the validation applications discussed in Chapter 4 of the Theory Manual. These are presented so the that the reader may have some example input files to use as a guide. Because of their length, computational mesh files have been omitted, but in the applications presented, the computational mesh files were generated with the `cartgrid` utility (Section 6.1) using the dimensions presented in the Theory Manual.

A.1 Subcritical, Uniform Flow in a Rectangular Channel

Section 4.1.1 of the Theory Manual presents a validation application for subcritical, uniform flow in a rectangular channel. This problem was solved using three computational mesh blocks. The upstream and downstream blocks were separated by a block with twice the resolution. This application demonstrates a relatively simple application that uses one-to-many cell block connections.

mass2.cfg

```
$Id: mass2_v027.cfg,v 1.2.2.1 2004/07/22 19:53:45 perk Exp $
MASS2 Test Case: Normal Flow with grid nesting
3           ! max number of blocks
2           ! max number of species
"grid1.dat"
"grid2.dat"
"grid3.dat"
T           ! on/off switch for hydrodynamics
F           ! on/off switch for transport calculations
F F "weather.dat"
F           ! extra debug printing
T           ! manning bottom friction equation
F   1728    ! write out restart files
F           ! read hotstart file
T           ! gage output
T F         ! initial: w.s. elev or depth, profile
04-01-1996 00:00:00  ! start date & time
04-01-1996 05:59:59  ! end date & time
60.0        ! time step (seconds)
12 10.0     ! hydro iterations, mass source error
2           ! scalar iterations
2           ! inner iterations for scalars
30          ! inner iterations for depth correction
0.20001 F   ! eddy viscosity
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
0.50001 F   ! diffusion coeff in eta (ft^2/sec)
```

```
0.02600 F   ! manning n value if manning=TRUE
1.49        ! constant in the bed shear stress
0.40        ! relaxation factor for depth corrections
0.0         ! not used
4.0         ! not used
0.2         ! initial uniform value of u velocity
0.0         ! initial uniform value of v velocity
25.0        ! initial uniform value of concentration
4.0         ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
F 0.0 0.0 0.0 ! do wet/dry, dry depth, rewet depth, zero depth
0.4 0.0 F 1 ! bed: porosity, initial depth, read initial, iterations
1   F       ! 2D output frequency, averaging
T T F       ! 2D enable netcdf, diag, flow
F F T 999999 ! cgns: enable, cell centered, field desc, times/file
1           ! gage output frequency
```

bcspecs.dat

```
1 US TABLE FLUX ALL "flow.dat" /
1 DS BLOCK ELEV ALL 2 /
2 US BLOCK VELO ALL 1 /
2 DS BLOCK ELEV ALL 3 /
3 US BLOCK VELO ALL 2
3 DS TABLE ELEV ALL "stage.dat" /
```

flow.dat

```
# $Id: flow.dat,v 1.2 2003/05/16 22:43:32 perk Exp $
01-01-1900 00:00:00   5000.0 /
01-01-2000 00:00:00   5000.0 /
```

stage.dat

```
# $Id: stage.dat,v 1.2 2003/05/16 22:43:34 perk Exp $
01-01-1900 00:00:00   5.0 /
01-01-2000 00:00:00   5.0 /
```

A.2 Two-Dimensional Flow Around a Spur Dike

Section 4.1.8 of the Theory Manual presents a validation test from the literature for two-dimensional flow around a spur dike. The shell script `mkgrid.sh` shown on page A.3 used the `cartgrid` to generate the single computational mesh block used in this application. The `mkgrid.sh` script generated the grid with metric dimensions, then converted to English. The spur dike was represented using a wall boundary condition (Section 4.3.3), as shown in the `bcspecs.dat` file on page A.4.

mkgrid.sh

```
#! /bin/sh
# ------------------------------------------------------------
# file: mkgrid.sh
# ------------------------------------------------------------
# ------------------------------------------------------------
# Battelle Memorial Institute
# Pacific Northwest Laboratory
# ------------------------------------------------------------
# ------------------------------------------------------------
# Created October  8, 2003 by William A. Perkins
# ------------------------------------------------------------

# dimensions in meters

L=5.4
W=0.9
nx=217
ny=37
dx=`echo scale=6\;$L/\($nx - 1\) | bc`
dy=`echo scale=6\;$W/\($ny - 1\) | bc`

../../../util/cart_grid/cartgrid <<EOF
$dx    ! longitudinal spacing
$dy    ! lateral spacing
$nx    ! downstream nodes
$ny    ! cross stream nodes
0.0    ! starting x coordinate
0.0    ! starting y coordinate

5.9014e-05 ! slope
0.0    ! downstream elevation
EOF

awk -f - grid.out > grid.dat <<EOF
NF == 5 {
  x = \$3/0.3048;
  y = \$4/0.3048;
  z = \$5/0.3048;
  printf("%5d %5d %12.6g %12.6g %12.6g\n", \$1, \$2, x, y, z);
  next;
}
```

```
{ print; }
EOF
```

mass2.cfg

```
$Id: mass2_v027.cfg,v 1.3.2.1 2004/07/22 19:53:44 perk Exp $
MASS2 Test Case: Two dimensional flow around a spur dike.
1           ! max number of blocks
1           ! max number of species
"grid.dat"
T           ! on/off switch for hydrodynamics
F           ! on/off switch for transport calculations
F F "weather.dat"
F           ! extra debug printing
T           ! manning bottom friction equation
T   100000  ! write out restart files
F           ! read hotstart file
T           ! gage output
T F         ! initial: w.s. elev or depth, profile
04-01-1996 00:00:00  ! start date & time
04-01-1996 00:05:00  ! end date & time
0.25        ! time step (seconds)
5 0.001     ! hydro iterations, mass source error
2           ! scalar iterations
2           ! inner iterations for scalars
25          ! inner iterations for depth correction
1.61e-02 F  ! eddy viscosity
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
0.50001 F   ! diffusion coeff in eta (ft^2/sec)
0.0100 F    ! manning n value if manning=TRUE
1.49        ! constant in the bed shear stress
0.20        ! relaxation factor for depth corrections
0.0         ! not used
0.62        ! not used
0.0         ! initial uniform value of u velocity
0.0         ! initial uniform value of v velocity
25.0        ! initial uniform value of concentration
0.62        ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
T 0.01 0.015 0.005 ! do wet/dry, dry depth, rewet depth, zero depth
0.4 0.0 F 1 ! bed: porosity, initial depth, read initial, iterations
999999 F    ! 2D output frequency, averaging
T T F       ! 2D enable netcdf, diag, flow
F F T 999999! cgns: enable, cell centered, field desc, times/file
4           ! gage output frequency
```

bcspecs.dat

```
 1 US TABLE FLUX ALL "flow.dat" /
 1 IN WALL  UVEL 73 1  6 /
 1 DS TABLE ELEV ALL "stage.dat" /
```

flow.dat

```
'  # Constant flow
   01-01-1900 00:00:00   1.5198 /
   01-01-3000 00:00:00   1.5198 /
```

stage.dat

```
'  # $Id: stage.dat,v 1.1 2003/10/24 20:00:35 perk Exp $
   01-01-1900 00:00:00    0.620 /
   01-01-3000 00:00:00    0.620 /
```

A.3 Lateral Mixing

This scalar transport application was presented in Section 4.2.3 of the Theory Manual. In this single block application, the hydrodynamic conditions were subcritical and uniform. The configuration file and hydrodynamics files are shown below. The transport of a single scalar was simulated; see the `scalar_source.dat` file on page A.7. Two concentrations were applied at the upstream boundary, as shown in the `scalar_bcspecs.dat` file on pageA.7.

A.3.1 Hydrodynamics Input Files

`mass2.cfg`

```
$Id: mass2_v027.base,v 1.4.2.1 2004/07/22 19:53:44 perk Exp $
MASS2 Test Case: Mixing of two streams
1           ! max number of blocks
1           ! max number of species
"grid.dat"
T           ! on/off switch for hydrodynamics
T           ! on/off switch for transport calculations
F F "weather.dat"
F           ! extra debug printing
T           ! manning bottom friction equation
F   1728    ! write out restart files
F           ! read hotstart file
T           ! gage output
T F         ! initial: w.s. elev or depth, profile
04-01-1996 00:00:00  ! start date & time
04-01-1996 05:59:59  ! end date & time
60.0        ! time step (seconds)
10 10.0     ! hydro iterations, mass source error
2           ! scalar iterations
2           ! inner iterations for scalars
50          ! inner iterations for depth correction
0.20001 F   ! eddy viscosity
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
3.00000 F   ! diffusion coeff in eta (ft^2/sec)
0.026 F     ! manning n value if manning=TRUE
1.49        ! constant in the bed shear stress
0.40        ! relaxation factor for depth corrections
0.0         ! not used
6.0         ! not used
0.2         ! initial uniform value of u velocity
0.0         ! initial uniform value of v velocity
0.0         ! initial uniform value of concentration
6.0         ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
F 0.0 0.0 0.0 ! do wet/dry, dry depth, rewet depth, zero depth
0.4 0.0 F 1 ! bed: porosity, initial depth, read initial, iterations
360 F       ! 2D output frequency, averaging
T T F       ! 2D enable netcdf, diag, flow
F F T 999999 ! cgns: enable, cell centered, field desc, times/file
```

```
10          ! gage output frequency
```

bcspecs.dat

```
1  1 US TABLE FLUX ALL "flow.dat" /
   1 DS TABLE ELEV ALL "stage.dat" /
```

flow.dat

```
1  # $Id: flow.dat,v 1.2 2001/11/29 18:16:00 perk Exp $
   01-01-1900 00:00:00   1000.0 /
   01-01-2000 00:00:00   1000.0 /
```

stage.dat

```
1  # $Id: stage.dat,v 1.2 2001/11/29 18:16:15 perk Exp $
   01-01-1900 00:00:00   6.0 /
   01-01-2000 00:00:00   6.0 /
```

A.3.2 Transport Input Files

scalar_source.dat

```
1  1 GEN stuff "Conservative transportable stuff" "bulldogs/liter" /
```

scalar_bcspecs.dat

```
1  1 US TABLE 1 CONC PART "conc.dat" 1  1 10 /
   1 US TABLE 1 CONC PART "bkgnd.dat" 1 11 20 /
   1 DS ZEROG 1 CONC ALL  /
```

bkgnd.dat

```
1  # $Id: bkgnd.dat,v 1.2 2001/11/29 18:15:59 perk Exp $
   01-01-1900 00:00:00  100.0 /
   01-01-2000 00:00:00  100.0 /
```

conc.dat

```
1  # $Id: conc.dat,v 1.2 2001/11/29 18:15:59 perk Exp $
   01-01-1900 00:00:00  200.0 /
   01-01-2000 00:00:00  200.0 /
```

Appendix B

Example Applications

Appendix B – Example Applications

In this appendix, several "real-world" applications of the Modular Aquatic Simulation System in Two Dimensions (MASS2) are described. This appendix is included to showcase some interesting MASS2 applications, provide examples of input files when interesting MASS2 features were used.

B.1 McNary Pool Dissolved Gas

As part of the U. S. Army Corps of Engineers' (USACE) Dissolved Gas Abatement (DGAS) Program, MASS2 was applied to the parts of the Columbia and Snake rivers impounded by McNary Dam, located on the Columbia River near Umatilla, Oregon. The application extended from Clover Island to McNary Dam on the Columbia River and from Ice Harbor Dam on the Snake River to its confluence with the Columbia River. Additional information on this application can be found in Richmond et al. (1999). The computational grid consisted of 13 blocks (Figure B.1) and covered over 78,000 acres, with an average resolution of 147 ft laterally and 330 ft longitudinally (Table B.1).

This application was developed to simulate the fate of total dissolved gas (TDG) generated at Ice Harbor Dam. It used the temperature and TDG simulation capabilities of MASS2. In the hydrodynamics, Ice Harbor Dam discharge was divided between spillway and power house, as shown in lines 1-2 of the `bcspecs.dat` file (page B.5). Several small spoil islands that were not resolved in the computational mesh were represented by an area with higher roughness, as shown in the `roughness_coeff.dat` file on page B.5.

Water that spills through the Ice Harbor Dam spillway entrains gas. The amount of entrainment was estimated. In `scalar_bcspecs.dat` (shown on page B.6), the boundary at the dam was split into two parts so different gas concentrations could be applied at the spillway and power house (lines 1 and 2). The same water temperature was applied over the entire dam boundary (line 10). Gas exchange coefficients (page B.6) were adjusted during calibration.

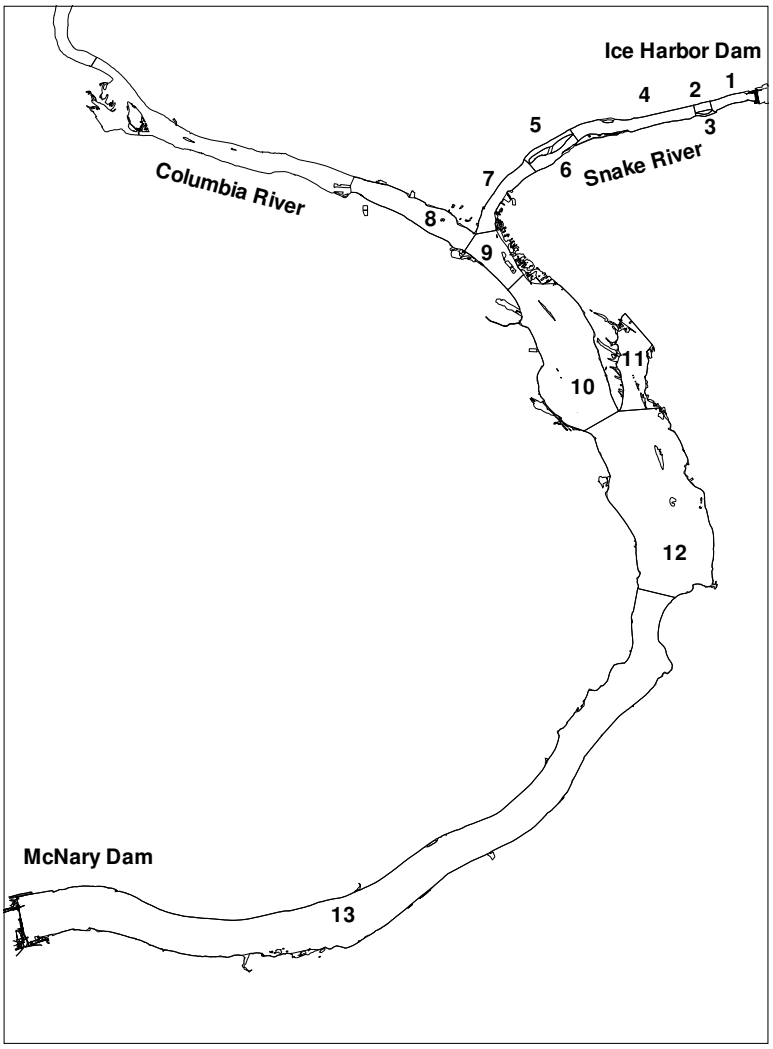


Figure B.1. Computational mesh block arrangement for the McNary Pool dissolved gas application.

Table B.1. Size and resolution statistics for the MASS2 computational grid for the McNary Pool dissolved gas application.

		Cell Size, feet						Block
		Lateral			Longitudinal			Area
Block	Cells	Min	Avg	Max	Min	Avg	Max	(acre)
1	1449	37	68	182	46	96	182	323
2	352	63	81	104	97	123	172	123
3	154	39	71	182	73	138	224	68
4	1701	61	88	210	76	221	375	1975
5	288	75	118	193	95	225	315	348
6	540	36	98	189	97	218	366	625
7	945	45	108	320	26	263	493	1662
8	1281	88	159	268	52	315	513	3041
9	1000	53	116	320	32	346	517	3285
10	2480	54	186	382	99	399	750	9973
11	1071	111	236	563	105	246	630	1615
12	4189	94	200	657	58	374	662	14418
13	12360	79	140	400	92	372	601	40569
all	27810	36	147	657	26	330	750	78024

mass2.cfg

```
mass2 version 0.27 configuration base file
FINS McNary Pool Simulation - Benchmark Simulation
13          max number of blocks
2           max number of species
"grid-3/grid-pt.013-1.dat"
"grid-3/grid-pt.000.dat"
"grid-3/grid-pt.001.dat"
"grid-3/grid-pt.002.dat"
"grid-3/grid-pt.003.dat"
"grid-3/grid-pt.004.dat"
"grid-3/grid-pt.005.dat"
"grid-3/grid-pt.006.dat"
"grid-3/grid-pt.007a.dat"
"grid-3/grid-pt.007b.dat"
"grid-3/grid-pt.009.dat"
"grid-3/grid-pt.008.dat"
"grid-3/grid-pt.010-all.dat"
T           ! on/off switch for hydrodynamics
T           ! on/off switch for transport calculations
T T "BCFiles/MCN_Weather.prn"
F           ! extra debug printing
T           ! manning bottom friction equation
F   18      ! write out restart files
T           ! read hotstart file
T           ! no gage output
T F         ! initial: w.s. elev or depth, profile
05-20-1997 12:00:00  ! start date & time
05-20-1997 16:00:00  ! end date & time
50.0        ! time step (seconds)
6 3000.0    ! hydro iterations, mass source error
2           ! scalar iterations
2           ! inner iterations for scalars
15          ! inner iterations for depth correction
0.20001 F   ! eddy viscosity
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
0.50001 F   ! diffusion coeff in eta (ft^2/sec)
0.027   T   ! manning n value if manning=TRUE
1.49        ! constant in the bed shear stress
0.40        ! relaxation factor for depth corrections
0.0         ! not used
338.3       ! not used
0.2         ! initial uniform value of u velocity
0.0         ! initial uniform value of v velocity
25.0        ! initial uniform value of concentration
338.3       ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
F 0.0 0.0 0.0 ! do wet/dry, dry depth, rewet depth, zero depth
0.4 0.0 F 1 ! bed: porosity, initial depth, read initial, iterations
72      F   ! 2D output frequency, averaging
T T F       ! 2D enable netcdf, diag, flow
T F T 999999! cgns: enable, cell centered, field desc, times/file
```

```
1           ! gage output frequency
```

bcspecs.dat

```
1 US TABLE FLUX PART "BCFiles/IHR_QS.prn" 1 10  /
1 US TABLE FLUX PART "BCFiles/IHR_QP.prn" 11 19 /
1 DS BLOCK ELEV PART 2 1 14 /
1 DS BLOCK ELEV PART 3 15 19 /
2 US BLOCK VELO ALL 1 /
2 DS BLOCK ELEV ALL 4 /
3 US BLOCK VELO ALL 1 /
3 DS BLOCK ELEV ALL 4 /
4 US BLOCK VELO PART 2 1 14 /
4 US BLOCK VELO PART 3 15 19 /
4 DS BLOCK ELEV PART 5 1 6 /
4 DS BLOCK ELEV PART 6 7 19 /
5 US BLOCK VELO ALL 4 /
5 DS BLOCK ELEV ALL 7 /
6 US BLOCK VELO ALL 4 /
6 DS BLOCK ELEV ALL 7 /
7 US BLOCK VELO PART 5 1 6 /
7 US BLOCK VELO PART 6 7 19 /
7 DS BLOCK ELEV ALL 9 /
8 US TABLE FLUX PART "BCFiles/zeroflow.dat" 1 9 /
8 US TABLE FLUX PART "BCFiles/Clover_Q.prn" 10 19 /
8 DS BLOCK ELEV ALL 9 /
9 US BLOCK VELO PART 8 1 19 /
9 US BLOCK VELO PART 7 20 38 /
9 DS TABLE VELO PART "BCFiles/zeroflow.dat" 24 38 /
9 DS BLOCK ELEV PART 10 1 23 /
10 US BLOCK VELO PART 9 1 23 /
10 US TABLE FLUX PART "BCFiles/zeroflow.dat" 24 38 /
10 DS BLOCK ELEV ALL 12 /
11 US TABLE FLUX ALL "BCFiles/zeroflow.dat" /
11 DS BLOCK ELEV ALL 12 /
12 US BLOCK VELO PART 10 1 38 /
12 US BLOCK VELO PART 11 39 57 /
12 DS TABLE VELO PART "BCFiles/zeroflow.dat" 39 57 /
12 DS BLOCK ELEV PART 13 1 38 /
13 US BLOCK VELO ALL 12 /
13 DS TABLE ELEV ALL "BCFiles/MCN_FBZ.prn" /
```

roughness_coeff.dat

```
 9 .045 14 21 24 29 /
```

scalar_source.dat

```
1 TDG  tdgconc      "Total Dissolved Gas"   "mg/l"  AIREXCH
       PARAMETERS   "gas_exchange_coeff.dat"    /
2 TEMP temperature  "Water Temperature" Celcius AIREXCH /
```

scalar_bcspecs.dat

```
  1 US TABLE 1 CONC PART "BCFiles/IHR_CS.prn" 1  1 10  /
  1 US TABLE 1 CONC PART "BCFiles/IHR_CP.prn" 1 11 19 /
  8 US TABLE 1 CONC ALL "BCFiles/Clover_C.prn" 1 /
  8 US ZEROG 1 CONC PART 1 9 /
  9 DS ZEROG 1 CONC PART 24 38 /
 10 US ZEROG 1 CONC PART 24 38 /
 11 US ZEROG 1 CONC ALL /
 12 DS ZEROG 1 CONC PART 39 57 /
 13 DS ZEROG 1 CONC ALL /
  1 US TABLE 2 CONC ALL "BCFiles/IHR_T.prn" 1 /
  8 US TABLE 2 CONC ALL "BCFiles/Clover_T.prn"  1 /
  8 US ZEROG 2 CONC PART 1 9 /
  9 DS ZEROG 2 CONC PART 24 38 /
 10 US ZEROG 2 CONC PART 24 38 /
 11 US ZEROG 2 CONC ALL /
 12 DS ZEROG 2 CONC PART 39 57 /
 13 DS ZEROG 2 CONC ALL /
```

gas_exchange_coeff.dat

```
 0.6885 -0.5025 0.1535 -0.0045 / a, b, c, d
```

B.2 Hanford Reach Hydrodynamics

In this application, MASS2 was used to simulate hydrodynamics in the Hanford Reach of the Columbia River. The simulated hydrodynamics were used to estimate juvenile fall Chinook habitat area and the portion of that area affected by rapid discharge fluctuations, as described by McMichael et al. (2003) and Perkins et al. (2004). MASS2 was configured to simulate approximately 23 miles of the Columbia River along the Hanford Reach from river mile (RM) 355 to 378. The computational mesh was composed of 16 blocks, as shown in Figure B.2, encompassed approximately 7800 acres, and used more than 224,000 cells (Table B.2). The grid resolution averaged 31 feet laterally and 49 feet longitudinally.

This MASS2 application is an example of using wetting and drying and using an initial water surface profile for the cold start simulation. The configuration file shown (page B.10) is that used for the initial cold start simulation. The cold start used an initial water surface profile simulated by a previously applied one-dimensional model (Perkins et al. 2002) and supplied to MASS2 in the `initial_specs.dat` file (page B.12). Hydrodynamic solution and wetting and drying parameters were varied as shown in Table B.3.

The boundary conditions required for MASS2 were total river discharge upstream and stage downstream. These were also supplied by the one-dimensional model which was used to simulate the Hanford Reach for the same periods as MASS2. The discharge and stage simulated by that model were extracted at the appropriate locations and used for MASS2 boundary conditions.

MASS2 was calibrated for the simulated region by adjusting the value of Manning's n until simulated stage closely matched the stage observed at three water level monitors operated by

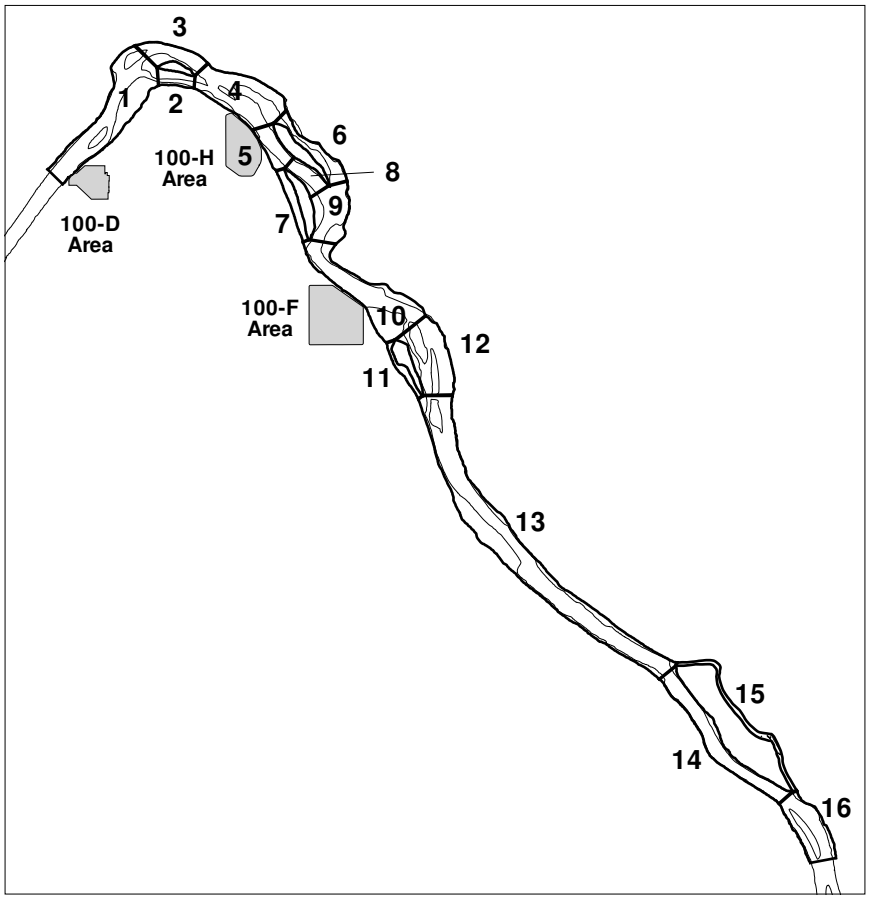


Figure B.2. Computational mesh blocks for simulation of Hanford Reach hydrodynamics.

the U.S. Department of Energy on the Hanford Reservation. The domain was divided into three areas between these stage monitors in which a single value of Manning's n was used (see the `roughness_coeff.dat` file on page B.13). The `gage_control.dat` file (page B.12) was used to specify the location of 10 stage recorder locations. One of these locations (ERC 100-D) became dry more often than the stage recorder, so an alternative location, farther in to the river, was also used. The gage location on line 7 was used to check that the downstream stage boundary conditions were appropriately applied.

Computationally, this was a relatively large problem, not just in space (i.e., number of cells) but also in time. This led to two problems while performing these multi-month simulations. The first was long execution time. On the fastest computers available to this work (Intel Pentium IV with clock speed greater than 2.0 gigahertz), it took about 6 to 8 hours to simulate a single day. This meant that simulating 60 days would have taken 15 to 20 days if such a processor were available for that length of time. The second problem was the space required to store hourly results. With the current MASS2 output options, a five-day simulation produced a results file that was too large for the computer system.

These problems were solved by dividing each simulation period into four-day periods. The simulation of each four-day period was started 12 hours early, allowing the simulation to transition

Table B.2. Size and resolution statistics for the MASS2 computational grid for the Hanford Reach hydrodynamics application.

		Cell Size, feet						Block
		Lateral			Longitudinal			Area
Block	Cells	Min	Avg	Max	Min	Avg	Max	(acre)
1	24120	19	34	111	22	53	86	1597
2	4641	22	27	37	26	40	56	172
3	4715	25	48	90	22	51	86	297
4	14400	18	39	83	25	53	88	977
5	4386	32	38	68	35	51	80	268
6	12300	13	29	60	18	29	82	255
7	3542	24	39	51	30	46	58	170
8	2821	42	58	74	32	46	58	135
9	9380	24	47	94	17	41	70	395
10	25110	14	29	95	22	45	83	1251
11	2318	14	30	55	37	53	70	152
12	8103	25	48	80	22	66	97	826
13	66870	14	27	73	22	49	87	3639
14	24095	13	19	31	23	56	70	1737
15	3263	20	36	71	37	76	117	433
16	14220	18	30	62	31	45	77	667
all	224284	13	31	111	17	49	117	7978

Table B.3. Parameters used for simulation of Hanford Reach hydrodynamics.

	Time Step (s)	Hydro. Iter.	Mass Src. Error (cfs)	Eddy Visc. (ft^2/s)	Under-relaxation	Dry Depth (ft)	Rewet Depth (ft)	Zero Depth (ft)
Cold start	1.0	3	3000.0	10.2	0.05	0.4	0.45	0.20
Warm up	15.0	15	3000.0	0.2	0.15	0.3	0.35	0.18
Simulation	16.0	12	8000.0	0.2	0.30	0.3	0.35	0.18
Simulation[(a)]	12.0	12	8000.0	0.2	0.30	0.3	0.35	0.18
Simulation[(b)]	10.0	12	8000.0	0.2	0.30	0.3	0.35	0.18

(a) Only used when simulations run with a 16.0 s time step became unstable.
(b) Only used when simulations run with a 12.0 s time step became unstable.

from starting conditions before simulation results were used. Several of these four-day periods were run simultaneously on several computers using the same starting conditions. In this way, the season simulation for a single scenario took about one week to complete, depending on the number and speed of available processors.

With this approach, the in-river area was simulated consistently, because of the 12-hour warm up. Simulated conditions within the river at the end of one four-day period matched those at the beginning of the next four-day period. However, the simulated time histories of any pools entrapped outside the river were not simulated consistently. One would expect the smaller entrapped pools to dry up over time due to evaporation and drainage. The rate at which these pools dry would be related to the weather, properties of their substrate material, and the distance from and height difference with the main river channel. Data to determine these drainage rates were not available. Given these complications, it was beyond the scope of this work to produce an accurate time history for pools outside the main river channel. Consequently, the time histories of pools outside were ignored in the analysis of simulation results.

mass2.cfg

```
mass2 version 0.25 configuration file
Grant County Stranding - Coarse Grid Setup, complete reach
16                      max number of blocks
2                       max number of species
"../grid/hanf50c-pt.000"  !  1
"../grid/hanf50c-pt.010"  !  2
"../grid/hanf50c-pt.009"  !  3
"../grid/hanf50c-pt.011"  !  4
"../grid/hanf50c-pt.001"  !  5
"../grid/hanf50c-pt.002"  !  6
"../grid/hanf50c-pt.003"  !  7
"../grid/hanf50c-pt.004"  !  8
"../grid/hanf50c-pt.005"  !  9
"../grid/hanf50c-pt.006"  ! 10
"../grid/hanf50c-pt.007"  ! 11
"../grid/hanf50c-pt.008"  ! 12
"../grid/hanf50c-pt.013"  ! 13
"../grid/hanf50c-pt.014"  ! 14
"../grid/hanf50c-pt.012"  ! 15
"../grid/hanf50c-pt.015"  ! 16
T           ! on/off switch for hydrodynamics
F           ! on/off switch for transport calculations
F F "./BCFiles/pasco_weather.prn"
F           ! extra debug output
T           ! manning bottom friction equation
T   3600    ! write out restart files
F           ! read hotstart file
T           ! no gage output
T T         ! initial: w.s. elev or depth, profile
03-01-2002 00:00:00      ! start date & time
03-01-2002 06:00:00      ! end date & time
1.0         ! time step (seconds)
2 3000.0    ! hydro iterations, mass source error
2           ! scalar iterations
5           ! inner iterations for scalars
25          ! inner iterations for depth correction
10.20001 F  ! eddy viscosity (ft^2/sec)
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
0.50001 F   ! diffusion coeff in eta (ft^2/sec)
0.025   F   ! manning n value if manning=TRUE
1.49        ! constant in bed shear stress
0.05        ! relaxation factor for depth corrections
0.0         ! not used
379.35      ! not used
0.5         ! initial uniform value of u velocity
```

```
0.0         ! initial uniform value of v velocity
25.0        ! initial uniform value of concentration
394.5       ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
T 0.40 0.45 0.20 ! do wet/dry, dry depth, rewet depth, zero depth
0.4 0.0 F 1 ! bed: porosity, initial depth, read initial, iterations
3600 F      ! 2D output frequency, averaging
F T F       ! 2D enable netcdf, diag, flow
T F T 999999 ! cgns: enable, cell centered, field desc, times/file
1           ! gage output frequency
```

bcspecs.dat

```
 1  US TABLE FLUX ALL  "./BCFiles/flow.dat" /
 1  DS BLOCK ELEV PART  2   1  49 /
 1  DS BLOCK ELEV PART  3  50  88 /
 2  US BLOCK VELO ALL   1 /
 2  DS BLOCK ELEV ALL   4 /
 3  US BLOCK VELO ALL   1 /
 3  DS BLOCK ELEV ALL   4 /
 4  US BLOCK VELO PART  2   1  49 /
 4  US BLOCK VELO PART  3  50  88 /
 4  DS BLOCK ELEV PART  5   1  49 /
 4  DS BLOCK ELEV PART  6  50  88 /
 5  US BLOCK VELO ALL   4 /
 5  DS BLOCK ELEV PART  7   1  20 /
 5  DS BLOCK ELEV PART  8  21  49 /
 6  US BLOCK VELO ALL   4 /
 6  DS BLOCK ELEV ALL   9 /
 7  US BLOCK VELO ALL   5 /
 7  DS BLOCK ELEV ALL  10 /
 8  US BLOCK VELO ALL   5 /
 8  DS BLOCK ELEV ALL   9 /
 9  US BLOCK VELO PART  8   1  29 /
 9  US BLOCK VELO PART  6  30  68 /
 9  DS BLOCK ELEV ALL  10 /
10  US BLOCK VELO PART  7   1  20 /
10  US BLOCK VELO PART  9  21  88 /
10  DS BLOCK ELEV PART 11  1 17/
10  DS BLOCK ELEV PART 12 18 88/
11  US BLOCK VELO ALL 10 /
11  DS BLOCK ELEV ALL 13 /
12  US BLOCK VELO ALL 10/
12  DS BLOCK ELEV ALL 13 /
13  US BLOCK VELO PART 11 1 17 /
```

```
13  US BLOCK VELO PART 12 18 88 /
13  DS BLOCK ELEV PART 14 1 77 /
13  DS BLOCK ELEV PART 15 78 88 /
14  US BLOCK VELO ALL 13/
14  DS BLOCK ELEV ALL 16/
15  US BLOCK VELO ALL 13 /
15  DS BLOCK ELEV ALL 16 /
16  US BLOCK VELO PART 14 1 77 /
16  US BLOCK VELO PART 15 78 88 /
16  DS TABLE ELEV ALL  "./BCFiles/stage.dat" /
```

initial_specs.dat

```
"Initial/p50b-pt.000"  / !  1
"Initial/p50b-pt.010"  / !  2
"Initial/p50b-pt.009"  / !  3
"Initial/p50b-pt.011"  / !  4
"Initial/p50b-pt.001"  / !  5
"Initial/p50b-pt.002"  / !  6
"Initial/p50b-pt.003"  / !  7
"Initial/p50b-pt.004"  / !  8
"Initial/p50b-pt.005"  / !  9
"Initial/p50b-pt.006"  / ! 10
"Initial/p50b-pt.007"  / ! 11
"Initial/p50b-pt.008"  /! 12
"Initial/p50b-pt.013"  /! 13
"Initial/p50b-pt.014"  /! 14
"Initial/p50b-pt.012"  /! 15
"Initial/p50b-pt.015"  /! 16
```

gage_control.dat

```
 1 167  83 "T54LBC piezometer" / T54LBC piezometer
 2  63  27 "T61IRC piezometer" / T61IRC piezometer
 4 117   9 "T64RBC piezometer" / T64RBC piezometer
12  38  47 "T81RBC piezometer" / T81RBC piezometer
13 228  51 "T90RBC piezometer" / T90RBC piezometer
13 451  15 "T94RBC piezometer" / T94RBC piezometer
14  24  63 "T101LBC piezometer" / T101LBC piezometer
16 155  40 "downstream extent" / downstream extent
1   22   7 "ERC 100-D" / ERC 100-D
4  115   9 "ERC 100-H" / ERC 100-H
10 116   9 "ERC 100-F" / ERC 100-F
1   22  10 "ERC 100-D Alternate" /
```

roughness_coeff.dat

```
1   1  0.0266    1 267  1 89
    2  0.0266    1  90  1 50
    3  0.0266    1 114  1 40
    4  0.0266    1 125  1 89
5   4  0.0278  126 159  1 89
    5  0.0278    1  85  1 50
    6  0.0278    1 299  1 40
    7  0.0278    1 160  1 21
    8  0.0278    1  90  1 30
10  9  0.0278    1 133  1 69
    10 0.0278    1 123  1 89
    10 0.0259  124 278  1 89
    11 0.0259    1 121  1 89
    12 0.0259    1 110  1 72
15  13 0.0259    1 741  1 89
    14 0.0259    1 304  1 78
    15 0.0259    1 250  1 12
    16 0.0259    1 157  1 89
```

B.3 System Assessment Capability Application

MASS2 is a component of the System Assessment Capability (SAC) (Kincaid et al. 2001). MASS2 is used to simulate the fate of radionuclides and other contaminants that have already or may enter the Columbia river from various sources on the U.S. Department of Energy Hanford Reservation. Because very long periods are simulated with SAC (1000 to 10,000 years), a coarse mesh was used. The computational mesh consisted of 57 blocks (Figure B.3) and about 4600 cells and covered about 18,000 acres (Table B.4). MASS2's transport-only mode was utilized to increase performance (at the expense of accuracy and completeness, perhaps).

Monthly mean discharges were used to provide the hydrodynamic conditions for transport only mode. In advance, the monthly mean discharge was simulated as a steady-state discharge for about 45 years of record. The hydrodynamic input files presented (Section B.3.1) are for one such monthly mean discharge.

In the transport input files (Section B.3.2), a single sediment fraction and the radionuclide Technetium-99 in dissolved and particulate phases were simulated (see the `scalar_bcspecs.dat` file on page B.24). A bed source is used to represent a source of Technetium-99 brought to the river through groundwater (lines 11 and 12 of `scalar_bcspecs.dat`). This was estimated with a groundwater flow and transport model. The groundwater model produced a contaminant and water flux at a number of locations. The same locations were used for both contaminant and water flux, which is why the same map file is used for both the `BEDSOURCE` (line 11) and `BEDFLOW` (line 12) records.

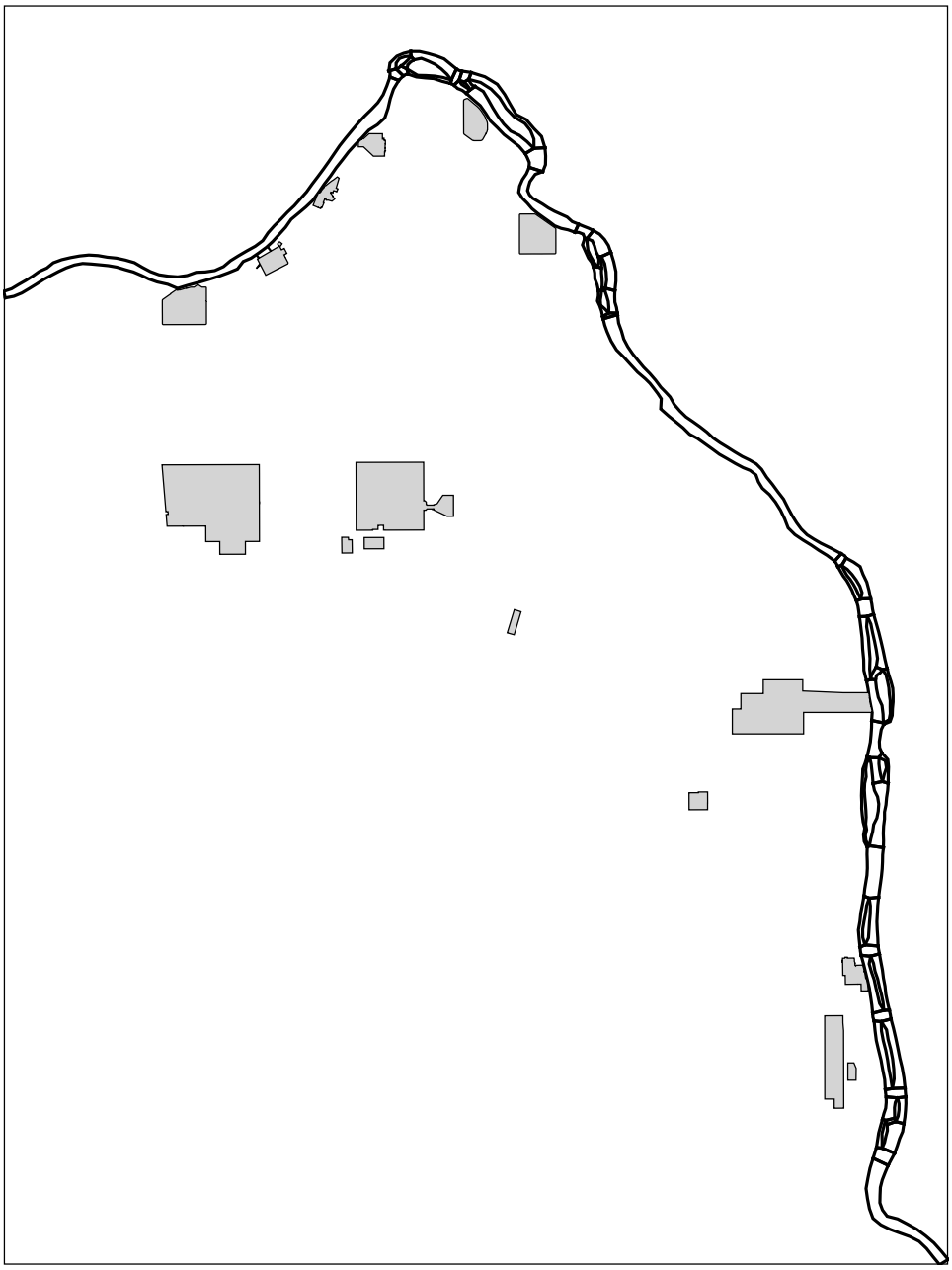


Figure B.3. Computational mesh block layout for the System Assessment Capability application.

Table B.4. Size and resolution statistics for the MASS2 computational grid.

		Cell Size, feet						Block
		Lateral			Longitudinal			Area
Block	Cells	Min	Avg	Max	Min	Avg	Max	(acre)
1	48	77	118	178	254	928	1371	1041
2	42	78	121	170	277	1035	1744	1192
3	30	116	159	210	420	708	1273	384
4	96	89	138	461	426	1017	1265	2424
5	64	129	167	469	277	644	1219	737
6	40	117	137	159	277	771	1395	634
7	40	166	209	947	362	756	2044	755
8	25	188	235	301	395	670	1395	334
9	77	99	183	286	661	1530	2056	4351
10	121	103	152	302	442	1251	1397	4519
11	35	80	136	189	637	854	1046	594
12	78	95	150	414	512	901	1409	1509
13	30	94	120	154	498	645	945	304
14	54	154	192	213	805	1163	1411	1716
15	54	103	142	501	236	723	927	689
16	42	69	129	226	147	699	941	506
17	20	87	105	116	236	552	1065	188
18	72	73	137	739	119	763	1391	1125
19	72	83	97	121	439	767	915	987
20	80	129	158	198	384	975	1228	1827
21	80	104	147	511	738	948	1542	1752
22	64	100	145	172	763	1390	1542	2920
23	80	98	139	655	604	1167	1414	2596
24	35	127	161	205	596	894	1439	727
25	55	58	140	188	831	978	1439	1230
26	91	100	135	457	644	1159	1542	2877
27	112	58	131	727	772	1012	1293	2667
28	80	82	139	214	796	946	1135	1652
29	48	158	196	216	846	967	1313	1046
30	42	66	118	165	794	1076	1313	1128
31	143	79	142	473	868	1028	1270	3478
32	144	103	156	481	876	1040	1221	3582
33	64	94	114	139	585	1104	1241	1828
34	80	120	163	227	537	1076	1165	2166
35	64	109	185	505	537	910	1217	1295
36	90	97	143	203	562	1066	1210	2434
37	72	99	153	220	580	1047	1176	1872
38	64	116	175	526	548	965	1404	1508
39	72	144	163	184	518	1225	1430	2657
40	90	121	163	220	630	1252	1444	3436
41	64	156	199	473	517	875	1444	1277
42	60	113	195	430	268	741	1036	798
43	48	154	181	204	640	910	1209	935
44	36	113	145	195	800	969	1038	780
45	24	284	304	329	245	615	1209	274
46	72	178	214	637	272	958	1188	1575
47	495	123	189	351	648	1313	1593	19746
48	64	83	138	563	254	798	1442	1177
49	80	101	176	663	687	1051	1681	2124
50	144	112	206	352	558	917	1271	2844
51	80	64	106	571	558	803	1031	1219
52	369	115	205	350	108	1200	1633	12677
53	144	174	250	356	800	1373	1555	6342
54	64	81	117	336	384	873	1618	1367
55	64	107	155	500	108	584	1214	712
56	64	158	182	375	800	1041	1483	1634
57	40	117	193	1099	265	561	1545	369
	4602	58	166	1099	108	1040	2056	18391

B.3.1 Hydrodynamics Input Files

mass2.cfg

```
mass2 version 0.25 configuration file
Checking block connections for Hanford Reach
57                       max number of blocks
2                       max number of species
"../new_sac_grid/sac_n-pt.001"
"../new_sac_grid/sac_n-pt.002"
"../new_sac_grid/sac_n-pt.003"
"../new_sac_grid/sac_n-pt.004"
"../new_sac_grid/sac_n-pt.005"
"../new_sac_grid/sac_n-pt.006"
"../new_sac_grid/sac_n-pt.007"
"../new_sac_grid/sac_n-pt.008"
"../new_sac_grid/sac_n-pt.009"
"../new_sac_grid/sac_n-pt.010"
"../new_sac_grid/sac_n-pt.011"
"../new_sac_grid/sac_n-pt.012"
"../new_sac_grid/sac_n-pt.013"
"../new_sac_grid/sac_n-pt.014"
"../new_sac_grid/sac_n-pt.015"
"../new_sac_grid/sac_n-pt.016"
"../new_sac_grid/sac_n-pt.017"
"../new_sac_grid/sac_n-pt.018"
"../new_sac_grid/sac_n-pt.019"
"../new_sac_grid/sac_n-pt.020"
"../new_sac_grid/sac_n-pt.021"
"../new_sac_grid/sac_n-pt.022"
"../new_sac_grid/sac_n-pt.023"
"../new_sac_grid/sac_n-pt.024"
"../new_sac_grid/sac_n-pt.025"
"../new_sac_grid/sac_n-pt.026"
"../new_sac_grid/sac_n-pt.027"
"../new_sac_grid/sac_n-pt.028"
"../new_sac_grid/sac_n-pt.029"
"../new_sac_grid/sac_n-pt.030"
"../new_sac_grid/sac_n-pt.031"
"../new_sac_grid/sac_n-pt.032"
"../new_sac_grid/sac_n-pt.033"
"../new_sac_grid/sac_n-pt.034"
"../new_sac_grid/sac_n-pt.035"
"../new_sac_grid/sac_n-pt.036"
"../new_sac_grid/sac_n-pt.037"
"../new_sac_grid/sac_n-pt.038"
"../new_sac_grid/sac_n-pt.039"
"../new_sac_grid/sac_n-pt.040"
```

```
"../new_sac_grid/sac_n-pt.041"
"../new_sac_grid/sac_n-pt.042"
"../new_sac_grid/sac_n-pt.043"
"../new_sac_grid/sac_n-pt.044"
"../new_sac_grid/sac_n-pt.045"
"../new_sac_grid/sac_n-pt.046"
"../new_sac_grid/sac_n-pt.047"
"../new_sac_grid/sac_n-pt.048"
"../new_sac_grid/sac_n-pt.049"
"../new_sac_grid/sac_n-pt.050"
"../new_sac_grid/sac_n-pt.051"
"../new_sac_grid/sac_n-pt.052"
"../new_sac_grid/sac_n-pt.053"
"../new_sac_grid/sac_n-pt.054"
"../new_sac_grid/sac_n-pt.055"
"../new_sac_grid/sac_n-pt.056"
"../new_sac_grid/sac_n-pt.000"
T           ! on/off switch for hydrodynamics
F           ! on/off switch for transport calculations
F F "../BCFiles/pasco_weather.prn"
F           ! extra debug printing
T           ! manning bottom friction equation
T   8400    ! write out restart files
T           ! read hotstart file
F           ! no gage output
F F         ! initial: w.s. elev or depth, profile
01-12-1975 12:00:00      ! start date & time
01-14-1975 23:59:59      ! end date & time
30.0        ! time step (seconds)
10 6000.0   ! hydro iterations, mass source error
2           ! scalar iterations
2           ! inner iterations for scalars
20          ! inner iterations for depth correction
0.20001 F   ! eddy viscosity
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
0.50001 F   ! diffusion coeff in eta (ft^2/sec)
0.029   F   ! manning n value if manning=TRUE
1.49        ! constant in the bed shear stress
0.4         ! relaxation factor for depth corrections
0.0         ! not used
355         ! not used
1.0         ! initial uniform value of u velocity
0.0         ! initial uniform value of v velocity
25.0        ! initial uniform value of concentration
395         ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
F 0.0 0.0 0.0 ! do wet/dry, dry depth, rewet depth, zero depth
```

```
0.4 0.0 F 1 ! bed: porosity, initial depth, read initial, iterations
999999  F   ! 2D output frequency, averaging
T F F       ! 2D enable netcdf, diag, flow
F F F 99999 ! cgns: enable, cell centered, field desc, times/file
5           ! gage output frequency
```

bcspecs.dat

```
47 US TABLE FLUX ALL "PRD-Flow.dat" /
47 DS BLOCK ELEV ALL 48 /
48 US BLOCK VELO ALL 47 /
48 DS BLOCK ELEV PART 57 1 8/
48 DS BLOCK ELEV PART 1 9 14/
57 US BLOCK VELO ALL 48/
57 DS BLOCK ELEV PART  2 1 4/
57 DS BLOCK ELEV PART 3 5 8/
1 US BLOCK VELO ALL 48 /
1 DS BLOCK ELEV ALL 4/
2 US BLOCK VELO ALL 57 /
2 DS BLOCK ELEV ALL 5 /
3 US BLOCK VELO ALL 57 /
3 DS BLOCK ELEV ALL 4 /
4 US BLOCK VELO PART 3 1 4 /
4 US BLOCK VELO PART 1 5 10 /
4 DS BLOCK ELEV ALL 5 /
5 US BLOCK VELO PART 2 1 4 /
5 US BLOCK VELO PART 4 5 14 /
5 DS BLOCK ELEV PART 6 1 6 /
5 DS BLOCK ELEV PART 7 7 14 /
6 US BLOCK VELO ALL 5 /
6 DS BLOCK ELEV ALL 10 /
7 US BLOCK VELO ALL 5 /
7 DS BLOCK ELEV PART 8 1 3 /
7 DS BLOCK ELEV PART 9 4 8 /
8 US BLOCK VELO ALL 7 /
8 DS BLOCK ELEV ALL 10 /
9 US BLOCK VELO ALL 7 /
9 DS BLOCK ELEV ALL 49 /
10 US BLOCK VELO PART 6 1 6 /
10 US BLOCK VELO PART 8 7 9 /
10 DS BLOCK ELEV ALL 49 /
49 US BLOCK VELO PART 10 1 9 /
49 US BLOCK VELO PART 9 10 14 /
49 DS BLOCK ELEV ALL 50 /
50 US BLOCK VELO ALL 49 /
```

```
50 DS BLOCK ELEV ALL 51 /
51 US BLOCK VELO ALL 50 /
51 DS BLOCK ELEV PART  11 1 3 /
51 DS BLOCK ELEV PART 12 4 14 /
11 US BLOCK VELO ALL 51 /
11 DS BLOCK ELEV ALL 15 /
12 US BLOCK VELO ALL 51 /
12 DS BLOCK ELEV PART 13 1 4 /
12 DS BLOCK ELEV PART 14 5 11 /
13 US BLOCK VELO ALL 12 /
13 DS BLOCK ELEV ALL 15 /
14 US BLOCK VELO ALL 12 /
14 DS BLOCK ELEV ALL 18 /
15 US BLOCK VELO PART 11 1 3 /
15 US BLOCK VELO PART 13 4 7 /
15 DS BLOCK ELEV PART 16 1 4 /
15 DS BLOCK ELEV PART 17 5 7 /
16 US BLOCK VELO ALL 15 /
16 DS BLOCK ELEV ALL 55 /
17 US BLOCK VELO ALL 15 /
17 DS BLOCK ELEV ALL 18 /
18 US BLOCK VELO PART 17 1 3 /
18 US BLOCK VELO PART 14 4 10 /
18 DS BLOCK ELEV ALL 55 /
55 US BLOCK VELO PART 16 1 4 /
55 US BLOCK VELO PART 18 5 14 /
55 DS BLOCK ELEV ALL 52 /
52 US BLOCK VELO ALL 55 /
52 DS BLOCK ELEV ALL 54 /
54 US BLOCK VELO ALL 52 /
54 DS BLOCK ELEV PART 19 1 6 /
54 DS BLOCK ELEV PART 20 7 14 /
19 US BLOCK VELO ALL 54 /
19 DS BLOCK ELEV ALL 21 /
20 US BLOCK VELO ALL 54 /
20 DS BLOCK ELEV ALL 21 /
21 US BLOCK VELO PART 19 1 6/
21 US BLOCK VELO PART 20 7 14 /
21 DS BLOCK ELEV PART  22 1 6/
21 DS BLOCK ELEV PART  23 7 14/
22 US BLOCK VELO ALL 21 /
22 DS BLOCK ELEV ALL 26 /
23 US BLOCK VELO ALL 21 /
23 DS BLOCK ELEV PART  24 1 5 /
23 DS BLOCK ELEV PART  25 6 8 /
```

```
24 US BLOCK VELO ALL 23 /
24 DS BLOCK ELEV ALL 26 /
25 US BLOCK VELO ALL 23 /
25 DS BLOCK ELEV ALL 27 /
26 US BLOCK VELO PART 22 1 6 /
26 US BLOCK VELO PART 24 7 11 /
26 DS BLOCK ELEV ALL 27 /
27 US BLOCK VELO PART 26 1 11 /
27 US BLOCK VELO PART 25 12 14 /
27 DS BLOCK ELEV PART 28 1 3 /
27 DS BLOCK ELEV PART 29 4 9  /
27 DS BLOCK ELEV PART 30 10 14 /
28 US BLOCK VELO ALL 27 /
28 DS BLOCK ELEV ALL 32 /
29 US BLOCK VELO ALL 27 /
29 DS BLOCK ELEV ALL 31 /
30 US BLOCK VELO ALL 27 /
30 DS BLOCK ELEV ALL 31 /
31 US BLOCK VELO PART 29 1 6 /
31 US BLOCK VELO PART 30 7 11 /  NEED TO CHECK!
31 DS BLOCK ELEV ALL 32 /
32 US BLOCK VELO PART 28 1 3 /
32 US BLOCK VELO PART 31 4 14 /
32 DS BLOCK ELEV PART 33 1 6 /
32 DS BLOCK ELEV PART 34 7 14 /
33 US BLOCK VELO ALL 32 /
33 DS BLOCK ELEV ALL 35 /
34 US BLOCK VELO ALL 32 /
34 DS BLOCK ELEV ALL 35 /
35 US BLOCK VELO PART 33 1 6 /
35 US BLOCK VELO PART 34 7 14 /
35 DS BLOCK ELEV PART 36 1 8 /
35 DS BLOCK ELEV PART 37 9 14 /
36 US BLOCK VELO ALL 35 /
36 DS BLOCK ELEV ALL 38 /
37 US BLOCK VELO ALL 35 /
37 DS BLOCK ELEV ALL 38 /
38 US BLOCK VELO PART 36 1 8 /
38 US BLOCK VELO PART 37 9 14 /
38 DS BLOCK ELEV PART 39 1 6 /
38 DS BLOCK ELEV PART 40 7 14 /
39 US BLOCK VELO ALL 38 /
39 DS BLOCK ELEV ALL 41 /
40 US BLOCK VELO ALL 38 /
40 DS BLOCK ELEV ALL 41 /
```

```
41 US BLOCK VELO PART 39 1 6 /
41 US BLOCK VELO PART 40 7 14 /
41 DS BLOCK ELEV PART 42 1 8 /
41 DS BLOCK ELEV PART 43 9 14 /
42 US BLOCK VELO ALL 41 /
42 DS BLOCK ELEV PART 44 1 4/
42 DS BLOCK ELEV PART 45 5 8 /
43 US BLOCK VELO ALL 41 /
43 DS BLOCK ELEV ALL 46 /
44 US BLOCK VELO ALL  42/
44 DS BLOCK ELEV ALL 56  /
45 US BLOCK VELO ALL  42 /
45 DS BLOCK ELEV ALL 46 /
46 US BLOCK VELO PART 45 1 4 /
46 US BLOCK VELO PART 43 5 10 /
46 DS BLOCK ELEV ALL 56 /
56 US BLOCK VELO PART 44 1 4 /
56 US BLOCK VELO PART 46 5 14 /
56 DS BLOCK ELEV ALL 53 /
53 US BLOCK VELO ALL 56 /
53 DS TABLE ELEV ALL "Steady_ZMCN.prn" /
```

PRD-Flow.dat

```
# Flow, cfs
01-01-1900 00:00:00  105093.548387097 /
01-01-2400 00:00:00  105093.548387097 /
```

Yakima-Flow.dat

```
# Flow, cfs
01-01-1900 00:00:00  5083.87096774194 /
01-01-2400 00:00:00  5083.87096774194 /
```

IHR-Flow.dat

```
# Flow, cfs
01-01-1900 00:00:00  38432.2580645161 /
01-01-2400 00:00:00  38432.2580645161 /
```

B.3.2 Transport Input Files

mass2.cfg

```
mass2 version 0.27 configuration file
SAC: Realization 1
57                        max number of blocks
3                        max number of species
"../new_sac_grid/sac_n-pt.001"
"../new_sac_grid/sac_n-pt.002"
"../new_sac_grid/sac_n-pt.003"
"../new_sac_grid/sac_n-pt.004"
"../new_sac_grid/sac_n-pt.005"
"../new_sac_grid/sac_n-pt.006"
"../new_sac_grid/sac_n-pt.007"
"../new_sac_grid/sac_n-pt.008"
"../new_sac_grid/sac_n-pt.009"
"../new_sac_grid/sac_n-pt.010"
"../new_sac_grid/sac_n-pt.011"
"../new_sac_grid/sac_n-pt.012"
"../new_sac_grid/sac_n-pt.013"
"../new_sac_grid/sac_n-pt.014"
"../new_sac_grid/sac_n-pt.015"
"../new_sac_grid/sac_n-pt.016"
"../new_sac_grid/sac_n-pt.017"
"../new_sac_grid/sac_n-pt.018"
"../new_sac_grid/sac_n-pt.019"
"../new_sac_grid/sac_n-pt.020"
"../new_sac_grid/sac_n-pt.021"
"../new_sac_grid/sac_n-pt.022"
"../new_sac_grid/sac_n-pt.023"
"../new_sac_grid/sac_n-pt.024"
"../new_sac_grid/sac_n-pt.025"
"../new_sac_grid/sac_n-pt.026"
"../new_sac_grid/sac_n-pt.027"
"../new_sac_grid/sac_n-pt.028"
"../new_sac_grid/sac_n-pt.029"
"../new_sac_grid/sac_n-pt.030"
"../new_sac_grid/sac_n-pt.031"
"../new_sac_grid/sac_n-pt.032"
"../new_sac_grid/sac_n-pt.033"
"../new_sac_grid/sac_n-pt.034"
"../new_sac_grid/sac_n-pt.035"
"../new_sac_grid/sac_n-pt.036"
"../new_sac_grid/sac_n-pt.037"
"../new_sac_grid/sac_n-pt.038"
"../new_sac_grid/sac_n-pt.039"
"../new_sac_grid/sac_n-pt.040"
```

```
"../new_sac_grid/sac_n-pt.041"
"../new_sac_grid/sac_n-pt.042"
"../new_sac_grid/sac_n-pt.043"
"../new_sac_grid/sac_n-pt.044"
"../new_sac_grid/sac_n-pt.045"
"../new_sac_grid/sac_n-pt.046"
"../new_sac_grid/sac_n-pt.047"
"../new_sac_grid/sac_n-pt.048"
"../new_sac_grid/sac_n-pt.049"
"../new_sac_grid/sac_n-pt.050"
"../new_sac_grid/sac_n-pt.051"
"../new_sac_grid/sac_n-pt.052"
"../new_sac_grid/sac_n-pt.053"
"../new_sac_grid/sac_n-pt.054"
"../new_sac_grid/sac_n-pt.055"
"../new_sac_grid/sac_n-pt.056"
"../new_sac_grid/sac_n-pt.000"
F           ! on/off switch for hydrodynamics
T           ! on/off switch for transport calculations
F F "../BCFiles/pasco_weather.prn"
F           ! extra debug printing
T           ! manning bottom friction equation
F   8400    ! write out restart files
F           ! read hotstart file
T           ! do gage output
F F         ! initial: w.s. elev or depth, profile
01-01-1944 00:00:00      ! start date & time
12-31-3051 23:59:59      ! end date & time
64800.0     ! time step (seconds)
10 5000.0   ! hydro iterations, mass source error
2           ! scalar iterations
2           ! inner iterations for scalars
25          ! inner iterations for depth correction
0.20001 F   ! eddy viscosity
0.20001 F   ! diffusion coeff in xsi (ft^2/sec)
0.00001 F   ! diffusion coeff in eta (ft^2/sec)
0.029   F   ! manning n value if manning=TRUE
1.49        ! constant in the bed shear stress
0.4         ! relaxation factor for depth corrections
0.0         ! not used
355         ! not used
1.0         ! initial uniform value of u velocity
0.0         ! initial uniform value of v velocity
0.0         ! initial uniform value of concentration
395         ! initial uniform value of depth OR w. s elev.
0.0         ! uniform value of u wind velocity
0.0         ! uniform value of v wind velocity
F 0.0 0.0 0.0 ! do wet/dry, dry depth, rewet depth, zero depth
```

```
0.4 0.0 T 6 ! bed: porosity, initial depth, read initial, iterations
487 F       ! 2D output frequency
F F F       ! 2D enable netcdf, diag, flow
T F F 100   ! cgns: enable, cell centered, field desc, times/file
487         ! gage output frequency
```

transport_only.dat

```
01-15-1943 00:00:00 "hydro/hotstart_01-15-1975_000000.bin" /
02-15-1943 00:00:00 "hydro/hotstart_02-15-1975_000000.bin" /
03-15-1943 00:00:00 "hydro/hotstart_03-15-1975_000000.bin" /
04-15-1943 00:00:00 "hydro/hotstart_04-15-1975_000000.bin" /
05-15-1943 00:00:00 "hydro/hotstart_05-15-1975_000000.bin" /
06-15-1943 00:00:00 "hydro/hotstart_06-15-1975_000000.bin" /
07-15-1943 00:00:00 "hydro/hotstart_07-15-1975_000000.bin" /
08-15-1943 00:00:00 "hydro/hotstart_08-15-1975_000000.bin" /
09-15-1943 00:00:00 "hydro/hotstart_09-15-1975_000000.bin" /
10-15-1943 00:00:00 "hydro/hotstart_10-15-1975_000000.bin" /
11-15-1943 00:00:00 "hydro/hotstart_11-15-1975_000000.bin" /
12-15-1943 00:00:00 "hydro/hotstart_12-15-1975_000000.bin" /
01-15-1944 00:00:00 "hydro/hotstart_01-15-1991_000000.bin" /
02-15-1944 00:00:00 "hydro/hotstart_02-15-1991_000000.bin" /
03-15-1944 00:00:00 "hydro/hotstart_03-15-1991_000000.bin" /
04-15-1944 00:00:00 "hydro/hotstart_04-15-1991_000000.bin" /
05-15-1944 00:00:00 "hydro/hotstart_05-15-1991_000000.bin" /
06-15-1944 00:00:00 "hydro/hotstart_06-15-1991_000000.bin" /
07-15-1944 00:00:00 "hydro/hotstart_07-15-1991_000000.bin" /
08-15-1944 00:00:00 "hydro/hotstart_08-15-1991_000000.bin" /
09-15-1944 00:00:00 "hydro/hotstart_09-15-1991_000000.bin" /
10-15-1944 00:00:00 "hydro/hotstart_10-15-1991_000000.bin" /
11-15-1944 00:00:00 "hydro/hotstart_11-15-1991_000000.bin" /
12-15-1944 00:00:00 "hydro/hotstart_12-15-1991_000000.bin" /
01-15-1945 00:00:00 "hydro/hotstart_01-15-1979_000000.bin" /
```

scalar_source.dat

```
1 SED "sediment" "Suspended Sediment" "kg/m^3"
    CONVERT 0.028317
    DENSITY 75.04
    D50  0.0001
    SETVEL      3.3e-05     DSHEAR  1.5e-03
    ERODIBILTY  0.0         ESHEAR  1.5e-03 /
2 GEN "Tc99" "Technetium-99" "Ci/m^3"
    CONVERT 0.028317
    HALFLIFE 213000.0
    DIFFUS   1e-07
```

```
      BEDSOURCE  "Tc99-list.dat" "cfestmap.dat"
      BEDFLOW "bedflow-list.dat" "cfestmap.dat" 35.315 /
   3 PART "Tc99-part" "Technetium-99 (Particulate Phase)" "Ci/m^3"
      CONVERT 0.028317
      DISSOLVED 2 SEDIMENT 1
      KD 1.000000E-04 BEDKD 1.000000E-10 RATE 1.0E-08 /
```

scalar_bcspecs.dat

```
47 US TABLE 1 CONC ALL  "bc/PRD-sediment.dat" 1 /
53 DS ZEROG 1 CONC ALL    /
47 US TABLE 2 CONC ALL  "bc/PRD-Tc99-diss.dat" 1 /
53 DS ZEROG 2 CONC ALL    /
47 US TABLE 3 CONC ALL  "bc/PRD-Tc99-part.dat" 1 /
53 DS ZEROG 3 CONC ALL    /
```

B.4 References

Kincaid CT, RW Bryce, PW Eslinger, CAB J. M. Becker, AL Bunn, CR Cole, EJ Freeman, GR Guensch, DG Horton, GV Last, TB Miley, WA Perkins, WE Nichols, M Oostrom, MC Richmond, DL Strenge, and PD Thorne. 2001. "Development of a Site-Wide System Assessment Capability." Presented at the Waste Management 2001 Symposium, February 25 - March 1, 2001, sponsored by the University of Arizona, Tuscon, Arizona.

McMichael GA, WA Perkins, CJ McMurray, YJ Chien, CL Rakowski, A Coleman, MC Richmond, J Vucelick, EV Arntzen, RP Mueller, CA Duberstein, and J Lukas. 2003. *Subyearling Chinook Salmon Stranding in the Hanford Reach of the Columbia River*. PNWD-3308, Battelle-Pacific Northwest Division, P.O. Box 999, Richland, Washington 99352. Prepared for Grant County Public Utility District No. 2.

Perkins W, M Richmond, and G McMichael. 2004. "Two-Dimensional Modeling of Time-Varying Hydrodynamics and Juvenile Chinook Salmon Habitat in the Hanford Reach of the Columbia River." In *Proceedings of the World Water and Environmental Resources Congress*. ASCE. Presented at conference held June 27-July 1 in Salt Lake City.

Perkins W, M Richmond, C Rakowski, A Coleman, and G Guensch. 2002. *Effects of Wanapum and Priest Rapids Impoundments on Columbia River Temperature*. PNWD-3269, Battelle Pacific Northwest Division, P.O. Box 999, Richland, Washington 99352. Prepared for Grant County Public Utility District.

Richmond M, W Perkins, and T Scheibe. 1999. *Two-Dimensional Hydrodynamic, Water Quality, and Fish Exposure Modeling of the Columbia and Snake Rivers. Part 1: Summary and Model Formulation.* Final Report, Battelle Pacific Northwest Division, P. O. Box 999, Richland, Washington, 99352. Prepared for the U.S. Army Corps of Engineers, Walla Walla District under Contract DACW68-96-D-0002.