STATE OF CALIFORNIA
THE RESOURCES AGENCY
DEPARTMENT OF WATER RESOURCES
Division of Planning

METHODOLOGY FOR
FLOW AND SALINITY ESTIMATES
IN THE
SACRAMENTO–SAN JOAQUIN DELTA AND SUISUN MARSH

FIFTEENTH ANNUAL PROGRESS REPORT
TO THE
STATE WATER RESOURCES CONTROL BOARD
in accordance with
Water Right Decision 1485, Order 9

June 1994
This is the fifteenth annual progress report on the development of methodologies to predict flow and salinity in the Sacramento–San Joaquin Delta and Suisun Marsh as required by Order 9 of the State Water Resources Control Board Water Rights Decision 1485. With D-1485 still in effect, the DWR Delta Modeling Section will continue to comply with Order 9 by filing this report. This document also serves the purpose of reporting activities under the Bay–Delta Evaluation Program, DWR Work Order 1463. This year, the report was compiled under the direction of Francis Chung, program manager of the Bay–Delta Evaluation Program. Presented below is a brief overview of the subjects addressed in this report. Contributing authors are noted in parenthesis.

**Ongoing Model Development: DWR Delta Simulation Model.** DWR's Delta Simulation Model, or DWRDSM, is the Department's main production tool for a variety of engineering analyses in the Delta. This year, development efforts were focused on the extension of model boundaries and on modifications to DWRDSM's flow submodel. These efforts will allow for a wider range of model applications while increasing numerical accuracy. The downstream tidal boundary was extended from Martinez to the Pacific Ocean at Golden Gate. The upstream Sacramento River boundary was extended from the American River confluence to Shasta Dam. (Mohammad Rayej and Parviz Nader-Tehrani)

**New Model Development: DSM2.** With the goal of creating a public domain model for the Delta, work on developing a new model herein referred to as Delta Simulation Model 2 or DSM2 has continued. The new model incorporates enhanced versions of the Four-Point flow submodel, the Branch Lagrangian Transport (BLTM) quality submodel, and other submodels and peripherals developed for DWRDSM. The target date for completing this task is June 1995. (Parviz Nader-Tehrani, Hari Rajbhandari, and Shawn Mayr)

**Particle Tracking Model for the Delta.** Fish and wildlife issues are critical to management of the Delta. Preliminary work on the Particle Tracking Model, a tool primarily designed to evaluate the transport of fish eggs and larvae, was reported in last year's progress report. Advances in model development, testing and verification were made this year and are reported. Significant developments include (1) a modification to quasi three-dimensionality that allows for particle tracking across channel width and depth, and (2) new subroutines that account for biological phenomenon such as the entrapment zone, egg and larvae mortality, and variable settling rates. (Tara Smith)

**Delta Island Consumptive Use (DICU) Analysis: Twitchell Island.** Recognizing the importance of agricultural activities on Delta hydrodynamics and water quality, a joint feasibility study to determine inflows and outflows from Delta islands is being conducted by DWR Division of Local Assistance and the U.S. Geological Survey. This study will focus on developing a water balance for Twitchell Island. The DICU model is currently being used by the study team in prioritizing data needs through the use of sensitivity analyses. One such sensitivity analysis is presented here. It is anticipated that the DICU model will be used to extrapolate knowledge gained from the Twitchell Island study to other islands in the Delta. (Nirmala Mahadevan)
**Disinfection By-Product Formation Modeling.** Work continued on developing, calibrating and validating a model of trihalomethane (THM) formation potential in Delta waters. Recent work, particularly in the areas of THM predictive equation calibration and DWRDSM performance testing, has focused on the anticipated joint use of DWRDSM and EPA's Water Treatment Plant (WTP) simulation program to look at cost-effective drinking water management alternatives. A formulation that can be used as a basis for predicting relative speciation of several disinfection by-products, including THMs, haloacetic acids, and haloacetonitriles, was also developed and is presented. (Paul Hutton)

**Delta Graphical User Interface (DGUI).** DGUI is used extensively to plot and manipulate observed and computed data pertaining to the Delta. This chapter reports new developments and additions to the DGUI. (Ralph Finch)

**Data Assembly: Time Series Data.** Efforts continued to further expand the data stored in-house. As of June 1994, the Section has assembled 12.2 million data points on flow, stage, velocity, gate position, water quality, etc. This represents an increase of about 50 percent from one year ago. It is anticipated that several other major sources of data will be assembled during the next year; these sources are discussed. (Ralph Finch)

**Model Input System.** A new input system is being developed to make DSM2 easy to use and to promote the execution of reliable model studies. Project status and future directions in the model input system are discussed in this chapter. (Ralph Finch)

**Refinement of Carriage Water Routine.** Several attempts were made to improve the performance of the existing routine, Minimum Delta Outflow (MDO), that is used to estimate the amount of carriage water. No conclusive findings are yet available. (Paul Hutton)

**Two Part Per Thousand Isohaline Equation Analysis.** EPA has proposed standards for the Delta estuary based on a flow–salinity relationship developed by Kimmerer and Monismith. Implementation of the proposed standard could have significant impacts on SWP operations. Therefore, a thorough review of the flow–salinity relationship was undertaken and is summarized in this chapter. (Chris Enright)
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Chapter 1

Ongoing Model Development:  
DWR Delta Simulation Model
**Introduction**

This year, development work on DWR's Delta Simulation Model (DWRDSM) included extending the model boundaries both in downstream and upstream directions as well as modifications to the flow submodel, DWRFLO. For more information about the model and past efforts in DWRDSM model development, the reader is referred to the 1990 through 1993 annual reports.

**Model Boundary Extension**

Currently, the DWRDSM network is bounded by the downstream tidal boundary at Martinez and the upstream river boundary at the confluence of the Sacramento and American rivers. However, as the need for planning and operational model studies have become more diversified, the current boundary locations may no longer be adequate. For example, the current tidal boundary at Martinez may provide boundary information for historic model studies. But for planning studies, boundary information may not be reliable or cumbersome to estimate. Relocating the tidal boundary from the interior of the estuary at Martinez to the Pacific Ocean has an added advantage of minimizing the boundary effects on areas in the vicinity of the boundary, e.g. the Suisun Marsh. The Delta Modeling Section and the Central District's Suisun Marsh Planning group have almost completed the boundary extension to Golden Gate.

There is also a need to extend the upstream river boundary currently at Sacramento (confluence of Sacramento and American rivers) to Shasta Dam. This is based on the need for temperature modeling of the water after release from the dam. Once the model boundary is extended and the network is established, a temperature routing module can be added. Then the model can be used to evaluate various reservoir release scenarios at different temperatures and water levels. After simulating the release, temperature loads beneficial for future salmon survival studies can be routed along the Sacramento River. By also accounting for temperature loads introduced by tributary inflows and agricultural return flows, simulation of reservoir releases will help us understand temperature variation along the river as the water travels downstream.
Golden Gate Boundary—The current downstream tidal boundary is at Martinez where available historic tide and salinity boundary information are adequate for model runs with historic boundary conditions. For planning model studies, however, a long-term average tide (19-year mean tide) and an estimate of salinity is used for model runs. Under these assumptions, the model can provide only average or typical information on flow and salinity conditions of the prototype. By relocating the downstream boundary to the ocean, we can use more realistic boundary information to perform studies with nonrepeating tides. This will enable us to use the model as a forecasting tool for future planning or operational studies.

a—Hydrodynamic Module: The model tidal boundary was extended from Martinez to the ocean at Golden Gate. The new Bay network required 128 additional channels, 86 junctions and 6 open water areas (Figure 1-1) bringing the Bay/Delta network to a total of 615 channels, 498 nodes and 19 open water areas. Hydrodynamic calibration of the Bay portion was performed using a few May 1988 tidal cycle data with the actual tidal boundary set at Golden Gate. Channel roughness coefficients between Golden Gate and Martinez were modified until the Golden Gate tide was propagated correctly, in phase and amplitude, to Martinez (Figure 1-2). The hydrodynamics module was verified by comparing model stage with measured stage at several interior Delta locations. Model results with the current boundary at Martinez were also included in the comparison and are shown in Figures 1-3 to 1-8.

To perform a full scale verification, the hydrodynamics module was verified with observed velocity and flow data. Verification results for velocity are in Figures 1-9 to 1-12 and for flow in Figures 1-13 to 1-16. Results show that the boundary extension to Golden Gate caused some phase shift in simulation results when compared with those simulated from the Martinez boundary. Also, it appears that simulations with the Golden Gate boundary resulted in lower water surface elevations in the interior Delta. This could be because the model lacks a baroclinic formulation. In general, the Golden Gate boundary extension produced stage, velocity and flow simulations that are consistent with field data as well as with the unmodified model.

b—Salinity Module: The salinity module of DWRDSM (with the boundary at Golden Gate) was calibrated and verified for Water Years 1987 through 1990. The first year was selected as a warm-up period. To generate flow information for salinity transport, the hydrodynamic module was run with a 19-year mean tide boundary at Golden Gate. The salinity boundary was set at constant ocean salinity of 35,000 ppm TDS throughout the simulation. Then the dispersion coefficients in channels between the Golden Gate and Martinez were modified until Golden Gate salinity was correctly dispersed to Martinez. Figure 1-17 shows model salinity, dispersed from Golden Gate to Martinez, against field measured salinity. While the model results do not depict the daily salinity fluctuations, due to use of the average 19-year mean tide, it generally follows the seasonal trend of salinity variations over the 1990 water year period. Salinity at some other locations beyond the current Martinez boundary, in the Suisun Marsh area such as S71, S72, S54 and C2 at Collinsville, are shown in Figures 1-18 to 1-21. The model results may be further improved by using daily varying hydrology and boundary tide.
Shasta Dam Boundary—The required channel geometry information for the Sacramento River, from I street to Shasta Dam, were obtained from the Hydrologic Engineering Center (HEC) office of Corps of Engineers (COE) in Davis, California. COE used a portion of the data for their HEC-5 model. Some data also were obtained from DWR, Northern District at Red Bluff, that were used in their river spawning gravel studies. One of the first steps was to reduce and align 32 aerial photos from 250 river miles from I street to Shasta Dam. Then channel boundaries were identified along with portions of the tributaries. A schematic network of river segments and connections was constructed by assigning numbers to channels and connections. A new model geometry (GEOM) input file was created and connected to an existing Bay/Delta file. This preliminary Shasta network has an additional 88 channels and 83 junctions bringing the total for the entire new Bay/Delta/Shasta network to 703 channels and 581 nodes. The channel geometry data should be modified, along with any necessary network adjustments, as new information becomes available.

When the GEOM input file was generated, an initial test run was made with DWRDSM’s hydrodynamic module. The model run indicated super-critical flow in upstream channels of the Shasta network. After some adjustments in channel dimensions, the model still had difficulties and was able to simulate only 5 hours of a 25-hour tidal cycle. This was probably due to DWRDSM’s explicit formulation (based on the method of characteristics), which could not handle rapidly varying and transitional flow in upstream reaches of the Sacramento River.

The Bay/Delta/Shasta network was then tested with the more robust DSM2 hydrodynamic model. DSM2 is discussed in Chapter 2. The DWRDSM geometry file was converted into an equivalent DSM2 file and, after making the necessary changes, DSM2 was run. The model simulated the entire tidal cycle with only minor adjustments in geometry. The only problem was the required CPU time (about 36 minutes on Sparc I and 20 minutes on Sparc II) to solve the large system of nonlinear flow equations iteratively. The CPU time was reduced to 14 minutes on Sparc II by renumbering the channels. Use of parallel processing may further reduce CPU time down to about 5 minutes per tidal cycle, the current time required by DWRDSM.
Figure 1-1. DWRDSM, San Francisco Bay Model Grid.
Figure 1-2

STAGE COMPARISON, DWRDSM VS FIELD DATA
Martinez, Channel 441

- Model Run - Golden Gate Boundary
- Field Data, E03290, May 1988

Stage in feet, MSL

Time in hours

--- - 200 250 300 350 400 ---
Figure 1-3
STAGE COMPARISON, DWRDSM VS FIELD DATA
San Joaquin River near Antioch, Channel 50

Stage in feet, MSL

Time in hours
Figure 1-4
STAGE COMPARISON, DWRDSM VS FIELD DATA
Middle River near East of Union Island, Channel 125
Figure 1-5
STAGE COMPARISON, DWRDSM VS FIELD DATA
Contra Costa Canal Intake, Channel 247
Figure 1-6
STAGE COMPARISON, DWRDSM VS FIELD DATA
Old River near Clifton Court Forebay, Channel 82

Stage in feet, MSL

Time in hours

- - - Model Run - Golden Gate boundary
- - - Model Run - Martinez Boundary
- - - Field Data, B95340, May 1988
Figure 1-7
STAGE COMPARISON, DWRDSM VS FIELD DATA
Middle River near Barrier, Channel 134

Stage in feet, MSL

Time in hours

- - - - - Model Run - Golden Gate boundary
- - - Model Run - Martinez Boundary
Field Data, B95500, May 1988
Figure 1-8

STAGE COMPARISON, DWRDSM VS FIELD DATA
San Joaquin River near Stockton, Channel 20
Figure 1-9

VELOCITY COMPARISON, DWRDSM VS FIELD DATA
San Joaquin River near Stockton, Channel 13
Figure 1-10

VELOCITY COMPARISON, DWRDSM VS FIELD DATA
San Joaquin River near Jersey Point, Channel 49

Field Data, May 1988
Figure 1-11

VELOCITY COMPARISON, DWRDSM VS FIELD DATA
Old River near Tracy Road, Channel 71

Velocity in fps

Time in hours

Golden Gate Boundary
Martinez Boundary
Field Data, May 1988
Figure 1-12

VELOCITY COMPARISON, DWRDSM VS FIELD DATA
Sacramento River near Decker Island, Channel 434
Figure 1-13
FLOW COMPARISON, DWRDSM VS FIELD DATA
San Joaquin River near Stockton, Channel 13

Time in hours
Flow in cfs
-4000
-3000
-2000
-1000
0
1000
2000
3000
4000
480 500 520 540 560 580

Golden Gate boundary
Martinez Boundary
Field Data, May 1988
Figure 1-14
FLOW COMPARISON, DWRDSM VS FIELD DATA
San Joaquin River near Jersey Point, Channel 49
Figure 1-15
FLOW COMPARISON, DWRDSM VS FIELD DATA
Old River near Tracy Road, Channel 71

Flow in cfs

-4000 -3000 -2000 -1000 0 1000 2000 3000 4000

Time in hours

480 500 520 540 560 580

Golden Gate Boundary
Martinez Boundary
Field Data, May 1988
Figure 1-16
FLOW COMPARISON, DWRDSM VS FIELD DATA
Sacramento River near Decker Island, Channel 434

--- Golden Gate Boundary
- Martinez Boundary
O Field Data, May 1988

Flow in cfs

Time in hours

480 500 520 540 560 580

0 50000 100000 150000 200000

-50000 -100000 -150000 -200000
Figure 1-17
Golden Gate Boundary, Martinez Salinity, Channel 441, Water Year 1990

Tidal Days

Salinity, ppm

- Model simulation
- Field data
Figure 1-18
Golden Gate Boundary, Montezuma Slough S71 Salinity, Channel 513, Water Year 1990

Salinity, ppm

Tidal Days

Model simulation
Field data
Figure 1-19
Golden Gate Boundary, S72 Salinity, Channel 530, Water Year 1990

Model simulation

Field data
Figure 1-20
Golden Gate Boundary, Montezuma Slough S54 Salinity, Channel 522, Water Year 1990

- Model simulation
- Field data

Tidal Days
Figure 1-21
Golden Gate Boundary, Collinsville Salinity, Channel 436, Water Year 1990

Salinity, ppm

Tidal Days

Model simulation
Field data
Modifications to the Flow Model

DWRFLO solves the momentum and continuity equations using an explicit technique, which is based on the method of characteristics. Due to the explicit nature of this method, continuity is enforced at junctions, but within a channel it is maintained only in an approximate sense. This leads to numerical leakage (or sometimes mass gain) in various channels, the magnitude of which may be small for a single channel but could add up to a considerable amount when accumulated over the whole Delta during the simulation (about 8 percent of the net delta outflow). An option was available in the original version of the DWRDSM, called the "Leak Plug", where the amount which was leaked would be added to the system, and the model is run for another tidal day. However, after this cycle, there is still some leakage (about 1 to 3 percent of net delta outflow) caused by the additional flow. A system was developed two years ago called the "Multiple Leak Plug", where the system goes through successive cycles, and during each cycle the leaked amount is added back to the system. The user either requests a certain number of Leak Plug cycles, or lets the model decide when to stop, based on a certain tolerance for the leakage amount (currently set at 100 cfs). Leakage can only be quantified for steady-state runs, where the change in storage in one tidal cycle is zero. For nonrepeating tides, the amount of leakage cannot be calculated, and thus the Leak-Plug option is not applicable; therefore these model runs suffer from this leakage problem.

DWRDSM was modified further by making adjustments to the calculated stage at the interior nodes. Figure 1–22 shows a rectangular channel of width B with one interior grid point. The prime (') notation indicates values at the future time step, which are computed using the method of characteristics.

![Figure 1-22. A Typical Channel with One Interior Grid Point](image-url)
The change of volume in one time step can be found two different ways:

1) Actual change in storage (trapezoidal rule)

\[ \Delta V = \left( \frac{Z_3' + 2Z_2' + Z_1'}{2} \right) - \left( \frac{Z_3 + 2Z_2 + Z_1}{2} \right) \times B \times \frac{\Delta x}{2} \]

2) Flow in minus flow out

\[ \Delta V = \left( \frac{Q_i + Q_i'}{2} \right) - \left( \frac{Q_2 + Q_2'}{2} \right) \times \frac{\Delta t}{2} \]

These two values should theoretically be equal. However they generally are not, thus creating a leakage. To eliminate leakage in this channel, the value of \( Z2' \) is adjusted by forcing these two expressions to be equal, leading to one equation one unknown. Test results indicate that the amount of correction for stage is usually less than 0.001 percent; however, this small modification results in elimination of leakage in this channel.

For channels with more than one intermediate grid point, the adjustments are done for the computed stage at all the intermediate points in the same proportion. For channels with no intermediate points, no adjustment can be made, and thus the leakage associated with them cannot be eliminated. Thus to reduce leakage, it would be desirable to force all channels to have an intermediate grid point. However, test results showed that some short channels suffered from Courant condition violation even for small flows. Reducing the time-step can help in this situation, however that results in higher CPU time.

Originally, the computational distance \( \Delta x \) for all the channels were selected based on a maximum velocity of 3 feet per second (fps), and 40 feet elevation. With this assumption, 202 (out of 496) channels had no intermediate grid point, i.e. 202 channels still have leakage problems. With an adjustment in the formula, the number of channels with no intermediate grid point was reduced to 60. This resulted in much lower leakage. Most test runs indicate that a leak–plug cycle may not even be necessary. The side–effect of making this adjustment is that the model has a higher chance of violating Courant condition. Test runs show that with the above adjustments, the model can handle up to about 50,000 cfs net delta outflow. To remedy this situation, instead of interrupting the model when a Courant condition violation was detected, the model is restarted, and the computational distance \( \Delta x \) is recalculated based on a maximum velocity of 5 fps. With this adjustment, the number of channels with no intermediate grid point is increased to 90. If the model still fails due to Courant condition violation, a final re–adjustment is performed based on a maximum velocity of 8 fps, increasing the number of channels with no intermediate grid point to 163. Previously, in a long–term modeling study, say a 20–year run, the user had to continuously keep track of the run. The remedy available to handle a Courant condition violation was to either reduce the time–step, or artificially increase the depth around the "problem" area. With the new code, the model makes all the necessary adjustments and restarts automatically. In addition the new code has a much better leakage characteristics.
Chapter 2

New Model Development: DSM2
The Delta Modeling Section is making continuous progress in developing DSM2, a public domain flow and transport model. DSM2 includes the "Four-Point" flow submodel and the "BLTM" (Branch Lagrangian Transport Model) submodel. These submodels were selected as alternate replacement for the current submodels. To learn more about the features and characteristics for each of these two submodels, the reader is referred to the Fourteenth Annual Progress Report (1993). This chapter outlines the efforts of the Delta Modeling Section in implementing the required modifications in these two submodels during the past year.

Flow Submodel: Four-Point

Four-Point is an implicit hydrodynamic model written by Delong and colleagues at the U.S. Geological Survey. The following describes the past year activities in model development. The Delta Modeling Section acknowledges the valuable guidance provided by Lew Delong.

Hydraulic Gates

The flow through a gate is calculated using the orifice flow equation:

\[ q = CA \sqrt{2g \Delta h} \quad (2-1) \]

where \( q \) is the flow through the gate, \( C \) is the gate flow coefficient, \( A \) is the flow area, and \( \Delta h \) is the hydraulic gradient between the two sides of the gate. Originally the gate formulation was developed using an explicit technique, where in a given iteration the flow through a gate was calculated based on the stage from a previous iteration. With this formulation in place, excessive numerical oscillations were observed around the gates. A filtering scheme was later introduced in an attempt to dampen out these oscillations:

\[ Q(t+1) = f \times q + (1 - f) Q(t) \quad (2-2) \]

where \( Q \) is the adjusted flow assigned to the channel, \( f \) is the filter coefficient \((0 < f < 1)\), \( q \) is the flow calculated from (Equation 2-1), and the index \( t \) represents the time step number. The filtering scheme managed to reduce the oscillations; however, it also produced an undesirable feature, due to an inherent phase lag between the flow calculated by (Equation 2-2) and the hydraulic gradient \( \Delta h \), introduced by filtering. For example, during a flow reversal, \( q \) will change its sign right away, but it takes some time for \( Q \) (which is the actual value used in the computations) to experience a change in sign, thus a phase lag results.
Lew Delong created a new feature in the code called "3 Parameter routine", which essentially makes it possible for gates to be modeled in an implicit form. To illustrate this routine, let's consider a junction with three connecting channels numbered 1 through 3. Q and Z denote flow and stage, respectively. The constraints, which must be enforced, are shown below:

\[
\begin{align*}
0_1 + 0_2 &= 0_3 \\
2_1 &= 2_2 \\
0_3 &= CA_j (Z_1 - Z_2) & \text{if } Z_1 > Z_2 \\
0_3 &= -CA_j (Z_3 - Z_1) & \text{if } Z_3 > Z_1
\end{align*}
\]

**Figure 2–1. Constraint Equations For A Typical Junction**

The same junction is considered again, this time a gate is placed at the upstream end of channel 3. The constraint equations will need to be modified as follows:

\[
\begin{align*}
0_1 + 0_2 &= 0_3 \\
Z_1 &= Z_2 \\
0_3 &= CA_j (Z_1 - Z_3) & \text{if } Z_1 > Z_3 \\
0_3 &= -CA_j (Z_3 - Z_1) & \text{if } Z_3 > Z_1
\end{align*}
\]

**Figure 2–2. Constraint Equations For A Gated Junction**
In an explicit formulation, \( Q_3 \) is calculated based on the stage at the previous iteration; however, this introduces oscillations as pointed out before. The "3 Parameter routine" enables the user to modify the matrix of coefficients to enforce the last equation shown above, relating the "3" variables \( Q_3, Z_1, \) and \( Z_3 \). Thus, this constraint is enforced implicitly. The results indicate that most of the oscillations are eliminated. Moreover, as no filtering is needed, undesirable phase lags are eliminated.

**Gate Scheduling**

The gate scheduling routine has been improved. All the gates can now be opened or closed at user-specified times, or once a user-specified condition is met. For example, Montezuma Slough Gate is sometimes instructed to open when the head gradient in the seaward direction is above a given value (say 0.3 ft), and close when the velocity during a flow reversal exceeds a given value (say 0.1 fps). The gate scheduling routine keeps track of all the gates and instructs the gate to open or close, once a triggering event has taken place. In addition, in order to avoid numerical oscillations induced by the sudden opening or closing of a gate, gates are allowed to open and close gradually, within a time specified by the user (say 20 minutes). This routine calculates a gate "time factor", shown by the letter \( F \), which is later multiplied by the calculated flow through the gate to give the adjusted flow. \( F \) will take value of 1 for a gate that is fully open, 0 when it is fully closed, and is interpolated between 0 and 1 when that gate is being opened or closed.

**Open Water Reservoir**

An open water reservoir is currently modeled as a storage tank, which can be connected to one or more channels either upstream or downstream. The flow out of a reservoir is calculated using a modified orifice equation:

\[
Q_{res} = C \sqrt{Z_{res} - Z_j}
\]  

(2–3)

where the \( C \) is the flow coefficient, \( Z_{res} \) is the reservoir stage, and \( Z_j \) is stage at the connecting junction. Originally open water areas were handled in an explicit form, where \( Q_{res} \) was calculated based on values of \( Z_{res} \) and \( Z_j \) from previous iteration. However, this created numerical oscillations (similar to hydraulic gates) thus requiring filtering, which in turn caused an undesirable phase lag. The model was modified to make it possible for the open water reservoirs to be simulated in an implicit form. To illustrate this point, consider a junction with two connecting channels. The constraint equations which must be enforced are:
Figure 2-3. Constraint equations for a junction with 2 channels

Now the same junction is considered, this time also connected to an open water reservoir. The constraint equations will then be modified as follows:

\[
\begin{align*}
Z_1 &= Z_2 \\
Q_1 &= Q_2 \\
Q_1 + Q_{res} &= Q_2 \\
Q_{res} &= C \sqrt{Z_{res} - Z_1} \text{ if } Z_{res} > Z_1 \\
Q_{res} &= -C \sqrt{Z_1 - Z_{res}} \text{ if } Z_1 > Z_{res}
\end{align*}
\]

Figure 2-4. Constraint equations for a junction with a reservoir
In an explicit formulation $Q_{\text{res}}$ is calculated based on the stage from previous iteration, thus causing numerical oscillation. Unfortunately the "3 parameter routine" cannot be used directly in this case in an implicit formulation, since $Z_{\text{res}}$ does not belong to the original list of unknowns, which included $Q$ (flow) and $Z$ (stage) at every computational point. To make this formulation fully implicit, one has to make room for the stage in every open water area in the list of unknowns, thus creating a major change in the way matrix entries are stored and the matrix is solved. The next best alternative is to implement the above equation in a semi-implicit form. $Q_{\text{res}}$ and $Z_{1}$ are handled implicitly, while $Z_{\text{res}}$ is handled explicitly. However, instead of actually using the value of $Z_{\text{res}}$ from the previous time step, an estimate for $Z_{\text{res}}$ is obtained from the following relationship:

$$Z_{\text{res}}(t+1)^* = Z_{\text{res}}(t) - Q_{\text{res}}(t) \Delta t / A_{\text{res}}$$  \hspace{1cm} (2-4)$$

where, $\Delta t$ is the time step, $A_{\text{res}}$ is the surface area of the open water reservoir, and the * notation represents an estimated value. This is the approach used in simulating open water reservoirs. The approach can be justified by taking advantage of the fact that stage in a reservoir does not change by much in one time step, which ordinarily is about 5 minutes.

**Pumping In and Out of the Open Water Areas**

Pumping is allowed to occur in and out of all of the reservoirs. To account for pumping Equation 2-4 is modified as follows:

$$Z_{\text{res}}(t+1) = Z_{\text{res}}(t) - [Q_{\text{res}}(t) + Q_{\text{pump}}(t)] \Delta t / A_{\text{res}}$$  \hspace{1cm} (2-5)$$

where $Q_{\text{pump}}$ is the amount of pumping (+ out of the reservoir). $Q_{\text{pump}}$ can easily be allowed to change with time.
Quality Submodel: Branch Lagrangian Transport Model

Progress has been made developing a model that can simulate the complex interaction of water quality variables to water resources managers in the Sacramento–San Joaquin Delta system. The water quality model is designed as part of the modified BLTM transport model which solves the convective–dispersive equations in a Lagrangian (moving) coordinate system. The reader is referred to the Fourteenth Annual Progress Report for a brief description of the BLTM Model.

The water quality model will have the capability to simulate the following variables:

1. arbitrary nonconservative constituent
2. carbonaceous BOD
3. dissolved oxygen
4. organic nitrogen
5. ammonia nitrogen
6. nitrite nitrogen
7. nitrate nitrogen
8. organic phosphorus
9. dissolved phosphorus
10. algae
11. temperature

The interaction among these parameters is shown in Figure 2−5. The conceptual and functional descriptions of constituent reactions represented in this model are based on two of the most commonly used water quality models, QUAL2E (Brown and Barnwell, 1987) and WQRRS (Smith, 1978). The distribution of state variables in space and time is computed by solving the following equation:

\[
\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[ D_x \frac{\partial C}{\partial x} \right] + k \ C + s
\]  

(2−6)

\( C \) = constituent concentration

\( D_x \) = longitudinal dispersion coefficient

\( k \) = first order rate constant

\( s \) = sources and sinks which are often functions of other constituent concentrations

The source and sink terms for simulated water quality parameters are described in the next section. Subroutines have been written for each constituent where the source and sink terms are computed at each time step.

A test run is in progress for a case when only a conservative constituent is simulated in the Delta. The code testing is in progress for the other constituents.
Figure 2-5. Interactions Among Water Quality Constituents
For heat exchange calculations, meteorologic data will be provided from NOAA consisting of air and wet bulb temperatures, wind speed, atmospheric pressure and cloudiness.

**Water Quality Model Parameters**

A nonconservative constituent may undergo a transformation of state, and its mass within the system may be changed by chemical, physical or biological processes. The rate of change of its concentration in water is usually a function of its concentration, environmental conditions including temperature, and concentrations of other constituents in the aquatic system. Reaction rates are usually represented by first order kinetics.

*Carbonaceous biochemical oxygen demand (CBOD).* The dissolved oxygen content of a pure natural water body would tend towards saturation if it were not for the presence of oxidizable organic matter. For the present study, CBOD is assumed to obey first order kinetics. The rate of change of CBOD can be expressed as:

\[
\frac{\delta L}{\delta t} = -k_1 L - k_3 L
\]

where

- \(L\) = CBOD concentration, mg/l
- \(k_1\) = CBOD decay rate at the ambient temperature, day\(^{-1}\)
- \(k_3\) = rate of loss of CBOD due to settling at the ambient temperature, day\(^{-1}\)

*Dissolved oxygen.* Dissolved oxygen (DO) is a major indicator of the general health of the aquatic ecosystem and is the most widely used water quality parameter. In an aquatic system, the sources of DO are:

- reaeration from the atmosphere
- photosynthetic oxygen production
- DO in incoming tributaries or effluents

Internal sinks of DO are:

- oxidation of carbonaceous organic matter
- oxidation of nitrogenous organic matter
- oxygen demand of sediments of water body
- oxygen use by aquatic plants
The rate of change in DO is computed by:

\[
\frac{\delta [O]}{\delta t} = - k_1 L + k_2 (O_s - [O]) - k_n[NH_3] \alpha_5 + (\alpha_3 \mu - \alpha_4 \varphi) [A] - \alpha_8 k_{ni}[NO_2] - \frac{k_4}{d}
\]  

(2-8)

where

- \([O]\) = dissolved oxygen concentration, mg/l
- \([NH_3]\) = ammonia concentration as N, mg/l
- \([NO_2]\) = nitrite concentration as N, mg/l
- \([A]\) = phytoplankton concentration, mg/l
- \(k_2\) = reaeration coefficient, day\(^{-1}\)
- \(k_n\) = ammonia decay rate at the ambient temperature, day\(^{-1}\)
- \(k_{ni}\) = nitrite decay rate at the ambient temperature, day\(^{-1}\)
- \(\mu\) = phytoplankton growth rate at the ambient temperature, day\(^{-1}\)
- \(\varphi\) = phytoplankton respiration rate at the ambient temperature, day\(^{-1}\)
- \(O_s\) = dissolved oxygen concentration at saturation, mg/l
- \(\alpha_5\) = amount of oxygen consumed in conversion of ammonia to nitrite
- \(\alpha_6\) = amount of oxygen consumed in conversion of nitrite to nitrate
- \(\alpha_3\) = amount of oxygen produced per unit of algal photosynthesis
- \(\alpha_4\) = amount of oxygen consumed per unit of algae respired
- \(K_4\) = benthic oxygen demand rate at the ambient temperature, g/ft\(^2\) day\(^{-1}\)
- \(d\) = mean channel depth, ft

**Phytoplankton.** As in most modeling efforts, phytoplankton population will be characterized as a whole by a measurement of the phytoplankton biomass present rather than considering the problem of different species and their associated environmental and nutrient requirements. Chlorophyll-\(a\) is a parameter characteristic of all phytoplankton and hence is used to describe the ensemble phytoplankton population. It is directly proportional to the concentration of phytoplanktonic algal biomass. The following expression is used in this study to convert algal biomass to chlorophyll-\(a\).

\[
Chl-a = \alpha_7[A]
\]  

(2-9)

where

- \(\alpha_7\) = a conversion factor, µg Chl-\(a\)/mg [A]
- \(Chl-a\) = chlorophyll-\(a\) concentration, µg/l

Phytoplankton increase by growth and decrease by respiration and settling. The rate of growth is determined using the limiting nutrient concept (either nitrogen or phosphorus). The rate of increases is computed by:

\[
\frac{\delta [A]}{\delta t} = [A](\mu - \varphi) - s_1 \frac{[A]}{d}
\]  

(2-10)
s_1 \quad = \quad \text{phytoplankton settling rate at ambient temperature, ft/day}

[A] \quad = \quad \text{phytoplankton concentration, mg/l}

\mu = \mu_{\text{max}} \cdot \text{FL} \cdot \min \left( \frac{N}{K_N + N}, \frac{P}{K_P + P} \right) \quad \quad \quad (2-11)

\mu_{\text{max}} \quad = \quad \text{maximum algal growth rate at the ambient temperature, day}^{-1}

N \quad = \quad \text{inorganic nitrogen concentration (NO3 + NH3), mg/l}

K_N \quad = \quad \text{nitrigen half saturation constant, mg/l}

K_P \quad = \quad \text{phosphorus half saturation constant, mg/l}

K_L \quad = \quad \text{half saturation constant for light, Kcal-m}^{-2} \cdot \text{s}^{-1} \text{ or Btu/ft}^2 \cdot \text{hr}

\text{(light intensity at which phytoplankton grows at half the maximum rate)}

FL \quad = \quad \text{algal growth limitation factor for light}

FL = (1/\lambda d) \ln \left[ \frac{K_L + I}{K_L + I e^{-\lambda d}} \right] \quad \quad \quad (2-12)

The above expression for FL is obtained when the variation of light intensity with depth represented by the relationship shown below is substituted in the Monod expression for light and integrated over the depth of flow.

I_z = I \exp (-\lambda z)

where

I \quad = \quad \text{light intensity at the surface, Kcal} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \text{ or Btu/ft}^2 \cdot \text{hr}

I_z \quad = \quad \text{light intensity at a given depth (z), Kcal} \cdot \text{m}^{-2} \cdot \text{s}^{-1} \text{ or Btu/ft}^2 \cdot \text{hr}

z \quad = \quad \text{depth variable, ft.}

\lambda \quad = \quad \text{light extinction coefficient, ft}^{-1}

The light extinction coefficient is usually defined as the linear sum of several extinction coefficients representing each component of light absorption (Bowie et al, 1985). The light extinction coefficient (\lambda) will be computed using the expression:

\lambda = \lambda_0 + \lambda_1 \alpha_7 [A] + \lambda_2 \left( \alpha_7 [A] \right)^{2/3} \quad \quad \quad (2-13)

where

\lambda_0 \quad = \quad \text{non-algal portion of the light extinction coefficient, ft}^{-1}

\lambda_1 \quad = \quad \text{linear algal self shading coefficient, ft}^{-1} \left( \text{\mu g- Chla/L} \right)^{-1}

\lambda_2 \quad = \quad \text{nonlinear algal self shading coefficient, ft}^{-1} \left( \text{\mu g- Chla/L} \right)^{-2/3}

\alpha_7 \quad = \quad \text{conversion factor, (\mu g- Chla/mg [A])}
**Nitrogen Series**

The differential equations representing transformations of organic nitrogen to ammonia, ammonia to nitrite, and nitrite to nitrate are shown below.

**Organic nitrogen**

\[
\frac{\partial [N - \text{org}]}{\partial t} = \alpha_1 [A] - k_{n - \text{org}} [N - \text{org}] - s_4 [N - \text{org}]
\]

where

- \([N - \text{org}] = \) concentration of organic nitrogen, mg/l
- \(k_{n - \text{org}} = \) rate constant for hydrolysis of organic nitrogen to ammonia nitrogen at the ambient temperature, day\(^{-1}\)
- \(\alpha_1 = \) fraction of algal biomass, which is nitrogen
- \(s_4 = \) organic nitrogen settling rate at the ambient temperature, day\(^{-1}\)

**Ammonia nitrogen**

\[
\frac{\partial [\text{NH}_3]}{\partial t} = k_{n - \text{org}} [N - \text{org}] - k_n [\text{NH}_3] + \frac{s_3}{d} - f \alpha_1 [A]
\]

where

- \(s_3 = \) benthic release rate for ammonia nitrogen at the ambient temperature, mg/ft\(^2\) day\(^{-1}\)
- \(f = \) fraction of algal uptake of nitrogen which is ammonia
- \(p = \) preference factor for ammonia nitrogen (0 to 1.0)

\[
p = \frac{[\text{NH}_3]}{[\text{NH}_3] + (1 - p)[\text{NO}_3]}
\]

**Nitrite nitrogen**

\[
\frac{\partial [\text{NO}_2]}{\partial t} = k_n [\text{NH}_3] - k_{ni} [\text{NO}_2]
\]

**Nitrate nitrogen**

\[
\frac{\partial [\text{NO}_3]}{\partial t} = k_n [\text{NO}_2] - (1 - f) \alpha_1 [A]
\]
**Phosphorus Series**

Organic forms of phosphorus are generated by the death of algae. These get transformed to the dissolved inorganic state, where it is available to algae for primary production.

**Organic Phosphorus**

\[
\frac{\partial [p - \text{org}]}{\partial t} = \alpha_2 [\alpha] - k_{p - \text{org}} [p - \text{org}] - S_5 [p - \text{org}]
\]  

(2-18)

where

- \([p - \text{org}] = \) concentration of organic phosphorus, mg/l
- \(\alpha_2 = \) fraction of algal biomass which is phosphorus
- \(k_{p - \text{org}} = \) organic phosphorus decay rate at the ambient temperature, day\(^{-1}\)
- \(S_5 = \) organic phosphorus settling rate at the ambient temperature, day\(^{-1}\)

**Dissolved Phosphorus**

\[
\frac{\partial [PO_4]}{\partial t} = K_{p - \text{org}} [PO_4] - \alpha_2 [\alpha] + \frac{S_2}{d}
\]  

(2-19)

where

- \([PO_4] = \) concentration of inorganic or dissolved phosphorus, mg/l
- \(S_2 = \) benthic release rate for dissolved phosphorus at the ambient temperature, mg/ft\(^2\) day\(^{-1}\)

**Arbitrary non-conservative or conservative constituent, arb**

\[
\frac{\partial [arb]}{\partial t} = - k_{arb} [arb] - S_6 [arb] + \frac{S_7}{d}
\]  

(2-20)

where

- \([arb] = \) concentration for the arbitrary constituent, mg/l
- \(S_6 = \) constituent settling rate at the ambient temperature, day\(^{-1}\)
- \(S_7 = \) benthic source for constituent at the ambient temperature, mg/ft\(^2\) day\(^{-1}\)
- \(k_{arb} = \) arbitrary constituent decay rate at the ambient temperature, day\(^{-1}\)

Equation 2-20 will work for a conservative constituent if the terms in the right side of the equation are made zero.
Heat Exchange at Air Water Interface

The heat exchange that occurs at the air–water surface is the dominant process controlling the heat budget for the water body. This exchange is controlled by the water temperature and meteorological conditions. The rate of energy transfer is computed as:

\[ Q_n = Q_{sn} + Q_{at} - Q_{ws} - Q_e + Q_h \]  

(2-21)

where

- \( Q_n \) = net heat energy transfer across the air–water interface, Btu/ft\(^2\)-hr
- \( Q_{sn} \) = net short wave solar radiation flux
- \( Q_{at} \) = net long wave atmospheric radiation flux
- \( Q_{ws} \) = water surface back radiation flux
- \( Q_e \) = evaporative heat flux
- \( Q_h \) = sensible heat flux

Net short wave solar radiation, \( Q_{sn} \). The net incoming solar radiation is short wave radiation which passes directly from the sun to the earth's surface. The attenuating effects of the absorption and scattering of the light in the atmosphere due to cloud cover and the reflection from the water surface must be considered in the computation of the solar radiation that penetrates the water surface. It may be represented by:

\[ Q_{sn} = Q_o a_t (1-0.65 C^2)(1-R_s) \]  

(2-22)

where

- \( Q_o \) = solar radiation intensity at the top of the atmosphere, a function of location and time, Btu/ft\(^2\)-hr
- \( Q_t \) = atmospheric transmissivity term
- \( C \) = cloud cover in tenths of sky covered, from 0.0 to 1.0
- \( R_s \) = reflectivity of the water surface, a function of the solar altitude, (a) of the form: \( R_s = A a^B \)

where \( a \) is the solar altitude in degrees and \( A \) and \( B \) are empirical constants.
New Model Development: DSM2

Net atmospheric radiation, $Q_{at}$. Some short-wave radiation from the sun plus radiation emitted by the ground or water surfaces enters the earth's atmosphere and is partly absorbed by water vapor, carbon dioxide, ozone and other atmospheric gases. These constituents, in turn, emit long wave radiation back to the ground and water surfaces, and outward to space. Such radiation is called atmospheric radiation. It is a function of absolute air temperature, cloudiness and water surface reflectivity (Orlob and Marjanovic, 1989).

A widely used formulation for approximating net atmospheric radiation is:

$$Q_{at} = C_{at} \sigma (T_a + 460)^4 (1 + 0.17C_a^2)(1 - R_a)$$

(2-23)

where

$C_{at} =$ Swinbank's coefficient approximately equal to $2.89 \times 10^{-6} \, \text{o} \, \text{R}^{-2}$

$\sigma =$ Stefan–Boltzmann constant $= 1.73 \times 10^{-9} \, \text{Btu/ft}^2\text{hr}^{0.5} \text{Rankine}^4$

$T_a =$ temperature of the radiating air mass, °F, at a level 6 feet above the water surface

$R_a =$ water surface reflectivity of long wave radiation $= 0.03$

Water surface back radiation, $Q_{ws}$. The loss of energy from a water body by long wave radiation is given by:

$$q_{ws} = \epsilon \sigma (T_s + 460)^4$$

(2-24)

where

$\epsilon =$ emissivity of the water surface, i.e., ratio of an actual radiation to that of a black body $= 0.97$

$T_s =$ water surface temperature, °F

Evaporative heat flux, $Q_e$

The evaporative heat loss occurs due to water changing a liquid state to a gas state (vapor) and the heat loss associated with the latent heat of vaporization.

$$Q_e = \gamma L_v E$$

(2-25)

where

$\gamma =$ specific weight of water, lb/ft$^3$

$L_v =$ latent heat of vaporization, Btu/lb

$E =$ evaporation rate, ft/hr, often expressed as $(a+bW) (e_s-e_a)$

where $a, b =$ constants and $W =$ wind speed, miles/hr, measured 6 feet above the water surface.

$e_s =$ saturation vapor pressure of the air, in. of Hg, at the temperature of the water surface, as given by

$e_s = 0.1001 \exp (0.03T_s) - 0.0837$
New Model Development: DSM2

\[ e_a = \text{water vapor pressure, in. of Hg, at a height of 6 feet above the water surface, given as} \]
\[ e_a = e_{wb} - 0.000367 \frac{P_a(T_a - T_{wb})}{1} \]

Other terms are as defined earlier.

\[ e_{wb} = \text{saturation vapor pressure, in. of Hg, at the wet bulb temperature} \]
\[ T_{wb} = \text{wet bulb temperature } ^\circ F \]
\[ P_a = \text{local barometric pressure, in. of Hg} \]

**Sensible heat flux, }Q_h.** Sensible heat is transferred between air and water by conduction and transferred away from the air–water interface by the same mechanisms as for evaporation. It is convenient to relate sensible and evaporative heat fluxes using Bowen's ratio in the form:

\[ Q_h = B q_e \]

where

\[ B = \text{Bowen's ratio} = 0.01 \frac{T_s - T_a}{P_a} \frac{e_s - e_a}{29.92} \]

Flood Modeling with DSM2

DSM2 has been proposed to replace the National Weather Service DWOPER–Network model. The purpose of the switch is to gain the many advantages of the Four-Point flow submodel and to consolidate the Section's model development and training efforts.

While DSM2 will ultimately represent an improvement in North Delta modeling technology, it must simulate flood events similarly to the way the National Weather Service DWOPER–Network does because it has long been the accepted tool for studying floods in the North Sacramento–San Joaquin Delta. Both models simulate unsteady flow by solving the St. Venant Equations in the implicit scheme. However, unlike the Network Model, DSM2 is very flexible for creating complex grids containing many branching channels while doing so with the Network model is more difficult.

**Feasibility Study**

To ensure that the two models give similar results, a series of feasibility tests were performed. First, a very simple grid (Figure 2–6) with 15 channels was configured with both computer models. An identical flood event was simulated with both models and the results were very similar. Following these promising results, a more complex grid with 40 channels and one reservoir was tested (Figure 2–7). Once again, similar results were observed. These preliminary tests, involving simple unsteady open channel flow and reservoir modeling, show that DSM2 could possibly be adapted for use as a flood model. Before more extensive tests can be performed, three key modifications must be made to DSM2.
**Tasks Required to Make DSM2 Capable of Simulating Flood Events**

Before DSM can duplicate a flood event with same degree of complexity as the Network model, three major modifications need to be completed:

1. **Code a New Grid** – A grid is needed that contains the same degree of complexity as the original DWOPER-Network Model for production model runs. The grid will have 118 cross sections.

2. **Modify Reservoirs** – The current reservoirs in DSM2 are too simple to accurately model islands and flood plain areas during flood events. Because the depth of water varies up to 10 feet during a flood event, the storage areas must reflect the varying amount of capacity for the range of levels experienced. The reservoirs will function similar to DWOPER-Network Model's polders and off-channel storage. There are two subsections of this task:
   a. Allow reservoir storage to vary with depth so that they can model complex islands and other off-channel storages such as flood plains.
   b. The DSM2 currently uses orifice flow to transfer water from channels to reservoirs. It is desirable to add a weir connection instead.

3. **Levee Breach Analysis**. The levee breach connection includes various triggering mechanisms. There are four types of trigger mechanisms for levee breaching:
   a. Time
   b. River Stage
   c. Reservoir (island) Stage
   d. River/Reservoir Stage Differential (This mechanism more realistically models levee stability.)

4. **Modify Internal Boundary Treatment**
   a. Allow the weir’s top-widths and culvert section area to vary with depth so that the internal boundary flow area can vary during the course of a flood.
   b. Combine weirs with culverts in the same cross-section in order to model important North Delta structures.

**DSM2 Calibration For Flood Modeling**

When the above features are added, DSM2 will be tested by simulating various historical flood events. The most important event to be simulated is the February 1986 flood event. Data from other flood events will also be obtained to increase the models reliability and to allow the model to be applied to a wide variety of flood events. Calibrating a model with only one flood event is not advisable. While a model may be able to simulate a certain event accurately, it may not be able to simulate other flood events of interest.
References


Chapter 3

Particle Tracking Model for the Delta
Particle Tracking Model for the Delta

The Particle Tracking Model simulates the transport and fate of individual particles within the Delta. The model was described in detail in the Fourteenth Annual Progress Report. This chapter will explain the developments of the model over the past year.

New Developments

Change to Quasi Three-Dimensional

Previously the model was quasi two-dimensional. In the quasi two-dimensional model, particles can move in either the x or z direction. In the model, the x direction is defined as lengthwise along the channel and the z direction is defined as the vertical direction. Each particle's movement is a function of the one-dimensional velocity in the channel. The average one-dimensional velocity given by the flow submodel, DWRFLO, is adjusted to reflect the vertical velocity profile. The vertical velocity profile provides velocities in the x direction that vary with the distance from the bottom. Movement in the x direction due to longitudinal dispersion is calculated using a dispersion coefficient and a random velocity component. This derived dispersion is a function of the stream's width, depth, and velocity and represents dispersion due to the transverse shear resulting from a transverse velocity profile. Movement in the z or vertical direction is due to vertical mixing which is a function of the water depth and velocity and is also due to the settling velocity of the particle.

In order to make the model quasi three-dimensional, the movement in the x direction due to the longitudinal dispersion coefficient and a random velocity component was replaced with movement due to a transverse velocity profile and transverse mixing (Bogle 1993). This modification allowed for the tracking of particles in the y direction or across the channel. The initial velocity profile adopted was a cosine function. The new profile is a quartic function and is still being implemented into the model (Bogle 1994). The dispersion due to the cosine velocity profile and the transverse mixing was verified against theoretical and observed dispersion.

X2 Boundary Option

Since the Particle Tracking Model is used to model biological species, a section of the program was modified to have the option of stopping particles from passing through the entrapment zone. The entrapment zone is represented by the 2 parts per thousand (ppt) salinity location. The 2 ppt salinity location is calculated using the Kimmerer/Monismith X2 equation. The node that represents the location closest to the X2 location is used as the boundary. Particles that encounter that node are not allowed to go past it towards the ocean.

Mortality

A new subroutine that provides for the elimination of particles in the system due to mortality was also written. The representative mortality rate used is for striped bass eggs and larvae. The rates were based on field data from the Department of Fish and Game (Miller 1992) and were given as a percentage loss over a time period. An exponential decay function and a random component was used to represent the loss of particles due to mortality.
Variable Settling Rates

A subroutine that allows for variable settling rates was added to the model. The settling rate is a function of the age and type of particle. Settling rates for striped bass eggs and larvae were used for the application. The settling rates used were based on laboratory results (Meinz and Heubach 1978). Eggs were given a constant settling rate and the settling rate for larvae varied linearly with time.

Testing and Verification

Dispersion Formulation

As stated previously, the particle tracking model's formulation was verified using longitudinal dispersion data. Data for various rivers (Fischer et al. 1979) was used for the verification. Table 3–1 shows the results of the verification. The goal of this verification was to see if by using average coefficients in the mixing equations the dispersion of particles (Column 6) would match well with the theoretical dispersion given by the equation shown in Column 5. These two columns show good agreement. The results were also compared to actual dispersion values shown in Column 4. There was not a clear agreement between model and observed values. This supported the fact that calibration of the model for the specific waterways of interest is necessary.

Ideally, the various mixing coefficients should be varied in order that the correct dispersion in particular channels is represented. However, since there is not adequate dispersion data to cover the delta at the present time, dispersion coefficients will remain the same for each individual channel.

Striped Bass Data: Travel Time and Vertical Distribution

Since a primary function of the model is to model the transport of biological species such as various species of fish eggs and larvae, an initial calibration of the model was done using Striped Bass eggs and larvae. Two sets of data were used to calibrate the model, travel time data and vertical distribution data.

The travel time calibration data consisted of continuous egg and larval samples taken at three locations in the Delta. This data is shown in Figure 3–1. This is an updated graph of the samples taken for the State Water Contractors (Hanson 1991). The samples taken at Bryte were used as the boundary condition and the model results were checked against the results at Courtland and Walnut Grove. The model used a real tide (historical stage at Martinez) and average inflows and outflows to model the hydrodynamics during the time period.
Experimental Measurements of Longitudinal Dispersion in Open Channels (p.126-127 in Fischer)

<table>
<thead>
<tr>
<th>Channel</th>
<th>Depth (ft)</th>
<th>Width (ft)</th>
<th>Mean vel (ft/s)</th>
<th>Observed K (ft^2/s)</th>
<th>K = 0.11u(w^2)/d</th>
<th>Model K</th>
</tr>
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<tr>
<td>(1) Chicago Ship Canal</td>
<td>26.48</td>
<td>160.11</td>
<td>0.89</td>
<td>32</td>
<td>94</td>
<td>107</td>
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<td>(2) Missouri River</td>
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<td>5.09</td>
<td>16153</td>
<td>27191</td>
<td>22837</td>
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<td>0.89</td>
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<td>160</td>
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<td>700</td>
<td>454</td>
<td>548</td>
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<td>(20) Comite River</td>
<td>1.41</td>
<td>52.50</td>
<td>1.21</td>
<td>151</td>
<td>261</td>
<td>241</td>
</tr>
<tr>
<td>(21) Sabine River</td>
<td>6.69</td>
<td>341.22</td>
<td>1.90</td>
<td>3392</td>
<td>3641</td>
<td>3090</td>
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<tr>
<td>(22)</td>
<td>15.58</td>
<td>416.69</td>
<td>2.10</td>
<td>7215</td>
<td>2573</td>
<td>2301</td>
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<tr>
<td>(23) Yadkin River</td>
<td>7.71</td>
<td>229.67</td>
<td>1.41</td>
<td>1185</td>
<td>1062</td>
<td>962</td>
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<tr>
<td>(24)</td>
<td>12.60</td>
<td>236.23</td>
<td>2.49</td>
<td>2800</td>
<td>1215</td>
<td>1181</td>
</tr>
</tbody>
</table>

Table 3-1
Bryte - Egg Concentration

Courtland - Egg Concentration

Walnut Grove - Egg Concentration

Figure 3-1
Figure 3-2 shows time series plots at Bryte, Courtland, and Walnut Grove. The three plots show observed data, model results, and model results with the mortality formulation. In the first plot, the observed data is input into the model. The model results shown are actually values 13,390 feet downstream of Bryte. This is why there is a slight lag between the model and observed values. For the other two plots the timing of the peaks match fairly well. By inputting an egg mortality rate of 50 percent over two days and a larval mortality rate of 14 percent per day, the amplitude of the peaks at Walnut Grove matched well. The peaks at Courtland did not match as well. C. Hanson indicated that the data collection conditions at Courtland were not as good as at the other two locations. Since there is a lower concentration of eggs/larvae at Courtland than at Walnut Grove, the amplitude of the peaks may have more to do with the data collection conditions than with the model results.

The U.S. Bureau of Reclamation collected vertical distribution data at five sites around the Delta Cross Channel in April 1990 (USBR 1990). Concentrations were measured at six locations within the cross section at each site. Figure 3-3 shows the results from one of the sampling periods. For the model simulations, daily average flows and the historical stage at Martinez were used as the input to the model. Particles were injected constantly throughout the simulation period. Top to bottom model distribution percentages were compared with the top to bottom percentage distribution of observed data. Differences in model results compared to observed data resulted in further investigation of the flow regime and the resulting distribution pattern. Measured flows in a few of the channels during this period match the timing and peaks of the flow model’s calculated flows. However, the observed distributions did not always match what is thought to happen when the flow changes. There is no strong correlation between the velocities in the channel and the top to bottom distribution. It is expected that the stratification would be greater with lower velocities, but this is not shown in the observed data. A better understanding of how the eggs/larvae were sampled might provide a greater insight into their distribution.

Sensitivity Testing

Various sensitivity tests were made with the model. One of the most important tested the effects of the time step on the results. Both mixing and settling are affected by the time step. The bigger the time step there is in the model, the farther the particle will travel during that time step. As an example, if a particle is settling at 0.0075 ft/s and there is a time step of 15 minutes, then the particle will fall 6.75 feet during that time step. If the time step is 5 minutes, the particle will fall 2.25 feet and for a one minute time step, 0.45 feet. The distance a particle moves due to mixing (both transverse and vertical) is also a function of the time step.
Bryte - No. of Eggs

Courtland Egg Concentrations

Walnut Grove Egg Concentrations

Figure 3-2
STRIPED BASS EGG + LARVA CONCENTRATIONS (#/m³)

- Walnut Grove
  - April 24, 1990
  - Sample Times: 09:55 - 11:00

- Delta Cross Channel
  - Tide Times:
    - Max Ebb: 10:35
    - Low Slack: 12:06

- Sacramento River above Delta Cross Channel
  - Sample Times:
    - SRAX: 09:55 - 11:00
    - SRBG: 09:50 - 10:52
    - SRBX: 11:07 - 12:06
    - DXC: 10:02 - 10:39
    - GSL: 11:15 - 11:27

- Sacramento River below Georgiana Slough
  - Sample Times:
    - 09:50 - 10:52

- Sacramento River below Delta Cross Channel
  - Sample Times:
    - 11:07 - 12:06

- Georgiana Slough
  - Sample Times:
    - 11:15 - 11:27

Figure 3-3
For a one minute time step, the particle will fall 0.45 feet. If the distances are added (assuming no mixing), after 15 minutes the particle should have fallen 6.75 feet, the same amount as during a 15 minute time step. A problem arises when the particle either reaches the top, bottom, or sides of the channel during the time step. If the particle reaches these boundaries it reflects back the additional distance it was to travel during that time step. If the time step is too big, the particle will be bouncing all over the channel (because during a larger time step a larger distance is traveled and there is a better chance of the particle reaching the boundaries of the channel). Because of this, the results from simulations with different time steps will be different. Results will be different even if mixing is the only mechanism for movement in the transverse and vertical direction and there is no settling. In this situation, for a large time step, the physical mixing process would not be modeled correctly. (Particles would still be encountering the boundaries of the channel.) A relationship that calculates the minimum time step needed for an accurate solution was developed by Gib Bogle. This relationship is a function of the velocity, width, and depth of the channel.

Test simulations were also done where velocity profiles and mixing were turned on and off. Several different hydrologies were used for the simulations and the tests provided a better understanding of the relative importance of each mechanism.

Other sensitivity tests include checking the effects of injecting different amounts of particles and changing the reflecting routine in the model. These tests also provided a better understanding of the impact of changing the various parameters.

**Sample Studies**

The model has been used to demonstrate the transport of particles under various hydrodynamic conditions. Two studies are briefly described here.

**QWEST and Transport**

A study was made evaluating the use of QWEST (the average daily flow traveling past Jersey Point) as a regulatory parameter in state and federal water project operations. The Particle Tracking Model was used to show that several different factors such as tide, advection, dispersion, and channel braiding affect the transport processes in the Delta.

**Effects of Pulse Flows and Export on Particle Transport**

Studies were made to examine the effects of pulse flows and exports on the transport of particles over an extended period of time. The studies provided a better understanding of the effect of pulse flows on the transport of particles under various hydrologies. As expected, pulse flows helped the movement of particles out to Suisun Bay if the particles were not located in the interior delta (south or below the San Joaquin River).
References


Chapter 4

Delta Island Consumptive Use Analysis: Twitchell Island
Agricultural water use data from Delta islands is needed to calculate the salt and organic contaminate loads entering the Delta channels from farming practices on each island. Therefore, DWR Division of Local Assistance and the U.S. Geologic Society are conducting a joint feasibility study to determine inflows and outflows from Delta islands. The plan is to study water use in the Delta by focussing on one island. Twitchell Island has been selected. After determining the water balance on Twitchell Island, extrapolation methods could be used to estimate the water balance on other Delta islands.

The Delta Island Consumptive Use (DICU) is used to help define the factors that dominate the water balance. The DICU model and associated routines were developed by DWR to estimate agricultural diversion and drainage volumes and salinity concentrations relative to DWRDSM nodes. This information is essential to studying flow and quality using models such as DWRDSM.

**DICU**

Figure 4-1 shows a simplified version of the water balance for a typical Delta Island used by the DICU model and associated routines. The DICU model is essentially a bookkeeping system (see Figure 4-2) which keeps track of water that enters, leaves, or is stored on each of 142 Delta subareas on a monthly time step. Factors such as precipitation, seepage, evapotranspiration (ET), irrigation, soil moisture storage, leach water, runoff, crop type, and acreage are used. The DICU model determines total consumptive use, consumptive use of precipitation, consumptive use of seepage, and consumptive use of applied water on each of the 142 subareas. Once this is done, an associated routine uses the results to calculate diversion and return flows for each subarea and allocates them to DWRDSM nodes (approximately 250 diversion nodes and 200 drainage nodes). The routine also assigns representative total dissolved solids and chloride concentrations to the nodal return flows. These results, in turn, are used as input to the DWRDSM model for verification and planning studies. Input to DICU includes:

- Acreage for 142 Delta subareas
- Acreage for 20 possible land use categories
- Noncritical and critical water year Delta land use
- Historic monthly total precipitation for 7 Delta stations (1922-1991)
- Historic monthly total pan evaporation (1956-1991)
- Mean ET for each land use category
- Estimated soil moisture accounting
- Typical monthly irrigation schedule for each irrigated crop and water year type
- Estimated schedule of monthly lowlands leaching/ponding
- Estimated irrigation efficiency
**Twitchell Island Diversion and Return Flow Estimates**

Twitchell Island is one of the 142 DICU subareas. The input data used for analyzing Twitchell Island consumptive use is displayed in Figures 4-3 to 4-5 and Tables 4-1 to 4-4.

Output data from DICU modeling is shown in Figures 4-6 through 4-10. Figure 4-6 shows monthly diversion and return flow estimates for Twitchell Island for water years 1970 through 1992 with a 70 percent irrigation efficiency. A database of similar values exists for water years 1922 through 1992 for each of the 142 Delta subareas. Figure 4-7 shows average, minimum and maximum monthly diversion and return flows over the period water year 1922-1992 (with a 70 percent irrigation efficiency). Figure 4-8 compares the information from Figure 4-6 to similar estimates generated with an irrigation efficiency of 50 percent. Figures 4-9 and 4-10 show the difference between average, minimum and maximum diversions and returns for a 50 percent versus a 70 percent irrigation efficiency. The plots show that changing the irrigation efficiency does have a significant impact in the summer months but not in the winter months. More details on sensitivity analysis tests are documented in a report soon to be released by the Delta Modeling Section.
Diversions = Seepage + Applied water + Leach water + Irrigation efficiency

Return = Precipitation + Drainage + Surface Runoff + Excess applied irrigation water

Precip Runoff = Precipitation - Total Consumptive Use (≥0)

Excess applied irrigation water = Required applied irrigation water / Irrigation efficiency - Required applied irrigation water

Figure 4-1. Water balance for a typical Delta Island.
Is the precip + seepage > ET demand?

- **Yes**: Use enough precip + seepage to satisfy the ET demand.
  - Is soil moisture at its upper limit?
    - **Yes**: Runoff = excess precip + seepage.
    - **No**: Is excess precip + seepage enough to raise soil moisture to its upper limit?
      - **Yes**: Runoff = excess precip + seepage minus amount needed to bring the soil moisture to its upper limit.
      - **No**: Excess precip + seepage is stored as soil moisture.
    - Is soil moisture above the lower limit?
      - **No**: Add applied water until the soil moisture is at its lower limit.
      - **Yes**: No applied water is needed.
- **No**: Use all precip + seepage to satisfy part of the ET demand.
  - Is soil moisture above the lower limit?
    - **Yes**: Deplete soil moisture to its lower limit and add applied water to satisfy the remaining ET demand.
    - **No**: Add applied water until the soil moisture is at its lower limit.
  - Is the excess soil moisture enough to satisfy the remaining ET demand?
    - **No**: No applied water is needed.
    - **Yes**: No applied water is needed.

Figure 4-2. DICU Model (soil moisture bookeeping).
Figure 4-3

Non-critical water year land use for Twitchell Island

- Alfalfa: 54%
- Pasture: 2%
- Grain: 11%
- Truck: 3%
- Safflower: 2%
- Corn: 3%
- Native vegetation: 2%
- Riparian vegetation: 5%

Critical water year land use for Twitchell Island

- Pasture: 49%
- Field: 12%
- Sugar beets: 6%
- Grain: 4%
- Truck: 3%
- Safflower: 2%
- Corn: 2%
- Native vegetation: 2%
- Riparian vegetation: 3%
Figure 4-4

DICU model annual ET per crop per unit area (inches)
Figure 4-5. Precipitation stations and Theissen Polygon boundaries.
Figure 4-6

Irrigation flows for Twitchell Island based on the DICU model (70% efficiency)

Divisions

Returns

Flow (cfs)


Flow (cfs)

Figure 4-7

Irrigation flows for Twitchell Island based on the DICU model (1922-1992) (70% irrigation efficiency)

**Diversions**

- Maximum
- Average
- Minimum

**Returns**

- Maximum
- Average
- Minimum

<table>
<thead>
<tr>
<th>Flow (cfs)</th>
<th>OCT</th>
<th>NOV</th>
<th>DEC</th>
<th>JAN</th>
<th>FEB</th>
<th>MAR</th>
<th>APR</th>
<th>MAY</th>
<th>JUN</th>
<th>JUL</th>
<th>AUG</th>
<th>SEP</th>
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<td>15</td>
<td>20</td>
<td>25</td>
<td>30</td>
<td>35</td>
<td>40</td>
<td>45</td>
<td>50</td>
<td>55</td>
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</tr>
</tbody>
</table>

Months: OCT, NOV, DEC, JAN, FEB, MAR, APR, MAY, JUN, JUL, AUG, SEP
Figure 4-8

Irrigation flows for Twitchell Island based on the DICU model

Divisions

Returns

Flow (cfs)

0 5 10 15 20 25 30 35 40 45 50 55


70% efficiency
50% efficiency
Figure 4-9
Diversions for Twitchell Island based on the DICU model (1922-1992) (50 vs 70% irrigation efficiency)

**Average diversion**

Minimum diversion

Maximum diversions
Drainage for Twitchell Island based on the DICU model (1922-1992) (50 vs 70% irrigation efficiency)

Average drainage

Minimum drainage

Maximum drainage
### Table 1
**DICU Model Input: Twitchell Island**
**Land Use Acreage and Seepage**

<table>
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<tr>
<th>Land use category</th>
<th>Land use acreage</th>
<th>Seepage (acre-ft)</th>
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</thead>
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<tr>
<td></td>
<td>Non-critical</td>
<td>Critical</td>
</tr>
<tr>
<td></td>
<td>water years</td>
<td>water years</td>
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<td>alfalfa</td>
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<td>114</td>
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<td>200</td>
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Seepage = (0.3 x root depth) x acreage

### Table 2
**DICU Model Total Monthly ET per Crop per Unit Area**

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<th>DEC</th>
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<th>FEB</th>
<th>MAR</th>
<th>APR</th>
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<th>JUN</th>
<th>JUL</th>
<th>AUG</th>
<th>SEP</th>
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<td>2.70</td>
<td>4.10</td>
<td>5.50</td>
<td>6.60</td>
<td>6.60</td>
<td>4.80</td>
<td>4.80</td>
<td>44.7</td>
</tr>
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<td>2.70</td>
<td>4.10</td>
<td>5.50</td>
<td>6.60</td>
<td>6.60</td>
<td>4.80</td>
<td>4.80</td>
<td>44.7</td>
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<td>1.70</td>
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<td>5.00</td>
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<td>2.70</td>
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**Delta Uplands**

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* Computed by multiplying soil depth by 3 inches per foot

* Computed by multiplying soil depth by 1.5 inches per foot

Lightly shaded area indicates limit of the critical water year irrigation season

Darkly shaded area indicates limit of the non-critical water year irrigation season
# Table 4

**Leach Water Volumes Based on George Sato’s 1981 Memo**

<table>
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<tr>
<th>Day</th>
<th>Flooded area derived from areal observations (acres)</th>
<th>Change in area flooded (acres)</th>
<th>Leach water adjustment (volume in AF, based on 2 ft water depth)</th>
<th>% of water applied/drained</th>
<th>% of lowlands area flooded</th>
<th>Leach water applied/drained (acre-ft)</th>
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<td>September 30</td>
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<td>0</td>
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<td>October 31</td>
<td>5,600</td>
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<td>+11,200</td>
<td>20% applied</td>
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<td>13,600</td>
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<td>30% applied</td>
<td>3.9%</td>
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<td>7.6%</td>
<td>+206</td>
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<td>January 31</td>
<td>11,800</td>
<td>-15,000</td>
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<td>56% drained</td>
<td>3.4%</td>
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<td>February 28</td>
<td>4,000</td>
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<td>29% drained</td>
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<td>March 30</td>
<td>300</td>
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<td>-7,400</td>
<td>14% drained</td>
<td>less than 1%</td>
<td>-58</td>
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<td>April 30</td>
<td>0</td>
<td>-300</td>
<td>-600</td>
<td>1% drained</td>
<td>0%</td>
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The volume of leach water assigned to each sub-area is based on the acreage of that sub-area divided by the total acreage flooded.

i.e. leach water applied to Twitchell Island leach in October = \((3580 \text{ acres} / 462000 \text{ acres}) \times 11200 \text{ AF} = 87 \text{ AF}\)
Chapter 5

*Disinfection By–Product Formation Modeling*
Work continued by Delta Modeling staff to develop, calibrate and verify a model of THM formation potential in Delta waters. Staff is working closely with DWR's Delta Planning Branch, members of the Municipal Water Quality Investigations committee, and Malcolm Pirnie Inc. (MPI) to explore Delta drinking water management alternatives through the coordinated use of DWRDSM and EPA's Water Treatment Plant (WTP) Simulation Program (MPI 1992). A proposal has recently been submitted to undertake such a task (MPI 1994).

The first section of this chapter presents a comparison between MPI's log-linear THM species equations, developed from an extensive Delta database, and an alternate formulation developed by Delta Modeling staff with the same database. The second section summarizes the status of an ongoing project to simulate historically-observed THM precursor transport in the Delta with DWRDSM. The final section presents a model that can be used as a basis for predicting relative speciation of several disinfection by-products, including THMs, haloacetic acids, and haloacetonitriles.

A Comparison With MPI's Delta THM Equations

Staff reviewed a report prepared by MPI on Delta THM modeling (MPI 1993) and comments are summarized in the subsequent text. Special attention was given to the calibration/verification database and on the THM predictive equations developed from this extensive Delta database. The conclusions and recommendations offered by Delta Modeling staff pertain only to the THM predictive equations and do not pertain to the overall EPA WTP Simulation Program developed by MPI.

MPI developed a set of predictive equations that are superior to their original "central-tendency" equations (Harrington et al 1992) for predicting THM formation in Delta waters. This conclusion is based on the following observations: (1) the new Delta THM equations were calibrated and verified with a large 900-point database covering a wide range of water qualities and representative chlorine dose-TOC ratios, (2) the new Delta THM equations employ more consistent usage of organic precursor variables, and (3) the new Delta THM equations generally include a term for raw water ammonia concentration.

Although MPI's new formulation works quite well for predicting total THMs, the equations dealing with individual THM species have some weaknesses which do not follow the observed chemistry of THM formation. For this reason, an alternate formulation to predict individual THM species within the overall WTP Simulation Program framework has been proposed by staff (DWR 1993). The proposed formulation employs the total THM predictive equation developed by MPI, the bromine distribution factor relationships developed by Hutton and Chung (1994), and a bromine incorporation factor equation calibrated and verified with the Delta database. Advantages of adopting the proposed formulation are listed below:

• The proposed formulation has fewer calibration requirements. MPI's formulation requires calibration of 36 constants while the proposed formulation requires calibration of only 10 constants.

• The proposed formulation gives individual species predictions that sum to the total THM prediction. MPI's THM species equations do not sum to the total THM prediction.
• The proposed formulation gives superior external verification results for all four of the individual THM species and gives internal verification results that are comparable to the MPI equations. See Figures 5-1(a) through 5-1(d).

• Sensitivity analyses show that some of the MPI equation responses are contrary to known chemical principles. For example, the MPI equations predict that total THM concentration (calculated from the sum of individual species) increases when chlorine dose decreases and when ammonia concentration increases. In contrast, the proposed formulation gives correct responses.

Figure 5-1 (a). Deviation Between Predicted and Observed Chloroform Concentrations: Comparison of External Verification

Figure 5-1 (b). Deviation Between Predicted and Observed Dichlorobromomethane Concentrations: Comparison of External Verification
Figure 5–1 (c). Deviation Between Predicted and Observed Chlorodibromomethane Concentrations: Comparison of External Verification

Figure 5–1 (d). Deviation Between Predicted and Observed Bromoform Concentrations: Comparison of External Verification
Historic Simulation of Delta THM Precursors

A modeling study was performed to validate the use of DWRDSM in simulating dynamic transport of organic and inorganic THM precursors in the Delta (DWR 1994). A simulation period of October 1983 through September 1992 was used. The analysis is partial because, while output results were obtained for several Delta locations, impacts were evaluated only at H.O. Banks–Delta Pumping Plant. As time permits, evaluation of impacts at other locations will be performed and model sensitivity will be explored. In this partial analysis, simulation approach and assumptions were outlined and results were compared with historically-observed data. Preliminary results from this study were presented at the ASCE National Hydraulic Engineering Conference in San Francisco (Hutton and Enright 1993).

A time series plot comparing observed and predicted dissolved organic carbon (DOC) is shown in Figure 5–2. Observed values are from DWR’s MWQI database. The model consistently underpredicts organic precursor concentrations; underprediction is particularly obvious for water years 1990–92. Delta Modeling staff hypothesized that DWRDSM is consistently underpredicting organic precursor concentrations because accurate information on agricultural diversion and drainage flows is not currently available. Agricultural drainage is thought to be the dominant source of organics in Delta water. DWR is working closely with USGS to measure diversion and drainage flows and to estimate previous flows from power consumption records.

![Figure 5-2. Predicted and Observed DOC Concentrations at Banks Pumping Plant: Water Years 1984–92](image-url)
Figure 5–3, which shows model estimates of relative organic precursor contributions from major tributary and in-Delta sources, suggests that the Sacramento River is the dominant source of organic precursor in Banks–Delta Pumping Plant water. According to the model, drainage contributions averaged 20 ± 9 percent over the entire simulation period. Drainage contributed up to 30–40 percent during summer irrigation and winter leaching peaks. Another DWR study estimated that agricultural drainage contributed approximately 40–50 percent of the total THM formation potential as carbon (TFPC) in the Delta during water year 1988 (DWR 1990). This difference in estimates is consistent with the hypothesis that DWRDSM is underpredicting organics because of inaccurate drainage information.

![Graph showing predicted contributions of DOC at Banks Pumping Plant: Water Years 1984–92](image)

**Figure 5–3. Predicted Contributions of DOC at Banks Pumping Plant: Water Years 1984–92**

**Relative Speciation of Disinfection By–Products: A General Model**

Delta Modeling staff investigated using a series of differential equations as a basis for predicting relative speciation of several drinking water disinfection by–products (DBPs). Model constants were successfully calibrated from several data sets to estimate relative concentrations of trihalomethanes (THMs), tri–and di–haloacetic acids, and dihaloacetonitriles. Relative distributions of trihaloacetic acid and THM species show remarkable similarity over the feasible range of bromine incorporation. Likewise, striking similarities exist between the relative distributions of dihaloacetic acid and dihaloacetonitrile species. Chemical formulas and acronyms used in this section are summarized in Table 5–1.
Table 5-1. DBP Nomenclature

<table>
<thead>
<tr>
<th>DBP Family</th>
<th>Compound</th>
<th>Acronym</th>
<th>Chemical Formula (Molecular Weight)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Trihalomethanes (THMs)</strong></td>
<td>Trichloromethane (Chloroform)</td>
<td>TCM</td>
<td>CHCl₃ (119.36)</td>
</tr>
<tr>
<td></td>
<td>Dichlorobromo-methane</td>
<td>DCBM</td>
<td>CHCl₂Br (163.82)</td>
</tr>
<tr>
<td></td>
<td>Chlorodibromo-methane</td>
<td>CDBM</td>
<td>CHClBr₂ (208.28)</td>
</tr>
<tr>
<td></td>
<td>Tribromomethane (Bromoform)</td>
<td>TBM</td>
<td>CBr₃ (252.74)</td>
</tr>
<tr>
<td><strong>Trihaloacetic Acids (THAAs)</strong></td>
<td>Trichloroacetic Acid</td>
<td>TCAA</td>
<td>CCl₃-COOH (163.38)</td>
</tr>
<tr>
<td></td>
<td>Dichlorobromoacetic Acid</td>
<td>DCBAA</td>
<td>CCl₂Br-COOH (207.83)</td>
</tr>
<tr>
<td></td>
<td>Chlorodibromoacetic Acid</td>
<td>CDBAA</td>
<td>CClBr₂-COOH (252.28)</td>
</tr>
<tr>
<td></td>
<td>Tribromoacetic Acid</td>
<td>TBAA</td>
<td>CBr₃-COOH (296.74)</td>
</tr>
<tr>
<td><strong>Dihaloacetic Acids (DHAAs)</strong></td>
<td>Dichloroacetic Acid</td>
<td>DCAA</td>
<td>CHCl₂-COOH (128.94)</td>
</tr>
<tr>
<td></td>
<td>Chlorobromoacetic Acid</td>
<td>CBAA</td>
<td>CHClBr-COOH (173.39)</td>
</tr>
<tr>
<td></td>
<td>Dibromoacetic Acid</td>
<td>DBAA</td>
<td>CBr₂-COOH (217.84)</td>
</tr>
<tr>
<td><strong>Dihaloacetonitriles (DHANs)</strong></td>
<td>Dichloroacetonitrile</td>
<td>DCAN</td>
<td>CHCl₂-CN (109.94)</td>
</tr>
<tr>
<td></td>
<td>Chlorobromoacetonitrile</td>
<td>CBAN</td>
<td>CHClBr-CN (154.50)</td>
</tr>
<tr>
<td></td>
<td>Dibromoacetonitrile</td>
<td>DBAN</td>
<td>CBr₂-CN (198.86)</td>
</tr>
</tbody>
</table>

**Governing Equations**

The governing differential equations are given below:

\[
\frac{dC_0}{dx} = -k_1C_0 \\
\frac{dC_1}{dx} = k_1C_0 - k_2C_1
\]  
(5-1)  
(5-2)
\[
\frac{dC_2}{d\tau} = k_2 C_1 - k_3 C_2 \\
\frac{dC_{n-1}}{d\tau} = k_{n-1} C_{n-2} - k_n C_{n-1} \\
\frac{dC_n}{d\tau} = k_n C_{n-1}
\]

where \( C_0, C_1, C_2, \ldots, C_{n-1}, \) and \( C_n \) denote molar concentrations of \( n \)-brominated DBPs at a level of bromine incorporation denoted by \( \tau \) and \( k_1, k_2, k_3, \ldots, k_{n-1}, \) and \( k_n \) are empirical constants. If \( k_1 \) is defined as unity and Equation 5–1 is solved, a definition for the dimensionless term \( \tau \) results:

\[
\tau = \ln \frac{C_0^{(0)}}{C_0}
\]

where \( C_0^{(0)} \) is the total molar concentration of the DBP family. If the bromine distribution factors are generalized to denote relative DBP species concentrations, then

\[
S = ( s_0(\tau), s_1(\tau), s_2(\tau), \ldots, s_{n-1}(\tau), s_n(\tau) )^T
\]

where vector elements are given by

\[
s_n(\tau) = \frac{C_n}{\sum_{n=0}^{n} C_n}
\]

and the solution of Equations 5–1 through 5–5 can be rearranged to obtain the following relationships:

\[
s_0(\tau) = e^{-k_1 \tau}
\]

\[
s_1(\tau) = \frac{k_1}{k_2 - k_1} e^{-k_1 \tau} + \frac{k_1}{k_1 - k_2} e^{-k_2 \tau}
\]

\[
s_2(\tau) = \frac{k_1 k_2}{(k_2 - k_1)(k_3 - k_1)} e^{-k_1 \tau} + \frac{k_1 k_2}{(k_1 - k_2)(k_3 - k_2)} e^{-k_2 \tau} + \frac{k_1 k_2}{(k_1 - k_3)(k_2 - k_3)} e^{-k_3 \tau}
\]
A bromine incorporation factor can be defined as the moles of bromine consumed by a DBP reaction per mole of total DBP formed:

\[
\eta = \frac{\sum_{n=0}^{n} nC_n}{\sum_{n=0}^{n} C_n}
\]  
(5-14)

This generalized definition of \( \eta \) can be expressed as a function of \( \tau \):

\[
\eta(\tau) = s_1(\tau) + 2s_2(\tau) + \ldots + (n-1)s_{n-1}(\tau) + ns_n(\tau)
\]  
(5-15)

To obtain uniform graphs for the course of DBP bromine substitution reactions, relative concentration (i.e. distribution factors) can be plotted versus \( \eta \). Such graphs can be generated over the feasible range of \( 0 \leq \eta \leq n \) by assigning different values to \( \tau \), substituting numerical values for the reaction rate constants into Equations 5-9 through 5-13, and calculating \( \eta \) according to Equation 5-15. From such graphs it is easy to
determine both the maximum relative concentration of a DBP compound and the value of \( \eta \) at which the maximum is reached. The same two values can be found directly from the assumed rate constants by setting the first derivatives of Equations 5-9 through 5-13 with respect to \( \tau \) equal to zero.

### Data Sets

Six data sets representing a wide range of observed and model-generated DBP species distributions are employed to calibrate model constants. Regression statistics are given in Table 5-2.

- **Polynomial Model-Generated Data (Data Set 1)** – Data Set 1 was generated by systematically substituting values of \( \eta \) between 0 and 3 (in increments of 0.01) into the polynomial model of Hutton and Chung (1994). This data set includes 301 vectors of THM species distribution data.

- **MWQI Data (Data Set 2)** – Data Set 2, reported by Hutton and Chung (1992), represents a high chlorine dose THM formation potential (THMFP) test that assays organic precursor levels in the Sacramento–San Joaquin Delta estuary. Prior to the test, samples are filtered through a 0.45 millipore membrane filter. Samples are then subjected to a fixed free chlorine dose of 120 mg/L and incubated for a seven day period at 25°C. Finally, the samples are dechlorinated using sodium thiosulfate and analyzed by the gas chromatograph purge and trap method. High chlorine doses are used to meet demands exerted by agricultural drain samples, waters which tend to contain exceptionally high levels of organic precursors. Samples are not buffered to a fixed pH value during the test. Data Set 2 contains 2024 observations of species distribution.

### Table 5-2. Regression Statistics for DBP Rate Constant Calibrations

<table>
<thead>
<tr>
<th>Data Set</th>
<th>DBP Family</th>
<th>No. (#) of Observations</th>
<th>( k_2 )</th>
<th>( r^2 )</th>
<th>( k_3 )</th>
<th>( r^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>THM</td>
<td>301</td>
<td>1.02 ± 0.007</td>
<td>0.97</td>
<td>0.49 ± 0.004</td>
<td>0.97</td>
</tr>
<tr>
<td>2</td>
<td>THM</td>
<td>2024</td>
<td>1.19 ± 0.010</td>
<td>0.93</td>
<td>0.54 ± 0.006</td>
<td>0.91</td>
</tr>
<tr>
<td>3</td>
<td>THM</td>
<td>1025</td>
<td>1.27 ± 0.007</td>
<td>0.98</td>
<td>0.64 ± 0.005</td>
<td>0.99</td>
</tr>
<tr>
<td>4</td>
<td>THM</td>
<td>333</td>
<td>1.23 ± 0.026</td>
<td>0.70</td>
<td>0.67 ± 0.020</td>
<td>0.76</td>
</tr>
<tr>
<td>5</td>
<td>THM</td>
<td>121</td>
<td>0.96 ± 0.012</td>
<td>0.89</td>
<td>0.47 ± 0.007</td>
<td>0.98</td>
</tr>
<tr>
<td>5</td>
<td>DHAA</td>
<td>42</td>
<td>0.97 ± 0.020</td>
<td>0.91</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>5</td>
<td>DHAN</td>
<td>84</td>
<td>0.76 ± 0.010</td>
<td>0.82</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>6</td>
<td>THM</td>
<td>69</td>
<td>1.19 ± 0.052</td>
<td>0.82</td>
<td>0.56 ± 0.050</td>
<td>0.43</td>
</tr>
<tr>
<td>6</td>
<td>THAA</td>
<td>72</td>
<td>0.95 ± 0.051</td>
<td>0.77</td>
<td>0.41 ± 0.026</td>
<td>0.79</td>
</tr>
<tr>
<td>6</td>
<td>DHAA</td>
<td>72</td>
<td>0.88 ± 0.027</td>
<td>0.91</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>
University of Arizona Data (Data Set 3) – Data Set 3 is a large THMFP data set developed at the University of Arizona by Amy et al. (1987). After each sample was filtered, a standard THMFP experiment was conducted under the following reaction conditions: a temperature of 20°C, a pH of 7, a chlorine-to-TOC ratio of 3.0, and a reaction time of 168 hours. In addition to the standard experiments, a series of kinetic experiments was conducted for each water sample to evaluate THM formation versus reaction time under varying reaction conditions of pH, temperature, chlorine dose and for incremental addition of bromide ion. Data Set 3 contains 1025 observations.

Miscellaneous THM Data (Data Set 4) – Data Set 4 represents a compilation of several data sets reported in the literature. This data set contains 333 observations that were generated under a wide range of raw water quality and reaction conditions.

SDS Data (Data Set 5) – Data Set 5 is a subset of a large simulated distribution system (SDS) database developed by the Metropolitan Water District of Southern California (MPI 1993). Data Set 5 includes THMs, DHAAs, and DHANs. THM and DHAN data in Data Set 5 were developed from an experimental protocol that employed jar treatment and filtration through granular media (Koch et al. 1991), while DHAA data were developed with a second protocol that employed filtration through a 0.45 µm pore filter (MPI 1993). Data Set 5 includes 121 THM observations, 42 DHAA observations, and 84 DHAN observations.

University of Cincinnati Data (Data Set 6) – Data Set 6 is a subset of experimental results produced at the University of Cincinnati by Pourmoghaddas (1990) and later reported by Pourmoghaddas et al (1993). The investigator studied the formation of mono-, di- and trihalogenated acetic acids, THMs, and DHANs by chlorinating a commercial humic acid at 25°C at two levels of chlorine, three levels of pH, four levels of bromide, and three reaction times. Data Set 6 includes 69 THM observations, 72 THAA observations, and 72 DHAA observations.

Comparisons Between Observed Data & Model Predictions

The proposed model shows a good fit to THM, THAA, DHAA, and DHAN relative species distribution data. Figures 5–4(a) through 5–4(c) show model predictions superimposed on DHAN data from Data Set 5.
Figure 5-4 (a) Relative Dichloracetonitrile Concentration as a Function of Bromine Incorporation Factor: Predicted and Observed Values

Figure 5-4 (b) Relative Chlorobromoacetonitrile Concentration as a Function of Bromine Incorporation Factor: Predicted and Observed Values
Figure 5-4 (c). Relative Dibromoacetonitrile Concentration as a Function of Bromine Incorporation Factor: Predicted and Observed Values
References


Chapter 6

Delta Graphical User Interface (DGUI)
The Delta Graphical User Interface (DGUI) is a program used on a Sun computer network to plot and manipulate observed and computed data pertaining to the Delta. The initial version of the DGUI was reported in 1992. This chapter reports about new developments of the DGUI and future directions.

Additional Features Added

Fourier Plot (Digital Filtering)

Any time series can be represented by a series of sinusoidal curves of differing frequency and amplitude. By converting a time signal to the frequency domain with a Fourier transform, removing or retaining desired frequencies, and then converting the signal back to the time domain, one can better see desired periodic components in the original data.

This plot consists of three windows: the original time series in the top window, the time series after filtering in the middle window, and the spectral density plot in the bottom window. In the bottom window, signal period (1/frequency) is on the x-axis, and signal strength on the y-axis.

The user can choose four types of filters: low-pass, high-pass, band-pass, and band-reject. Low pass means to enhance frequencies lower than the specified cutoff (long periods), while high-pass will enhance frequencies higher than the specified cutoff. In the band-pass filter, the user specifies two cutoff values and the filter enhances those frequencies between the two values; in band-reject, the filter attenuates frequencies between the two cutoff values.

Cutoff values are set by moving the mouse around the bottom window until the desired period is displayed, then clicking the button. This simple procedure is repeated for the band filters. Then the filter is calculated and the resulting signal displayed in the middle window. As with other filtering operations in the DGUI, the results may be sent to the printer, or stored in a new pathname and written to a file.

Figure 6–1 shows an example of this plot, using two months of stage data at Martinez. A low-pass filter was selected, with the cutoff period at about 30 hours. This produces a filtered signal without the daily tide variations, but with the spring–neap cycle and other long-term variations.

Additional work to this plot will involve the use of alternate algorithms for data that is irregularly sampled or that has missing values.

Axis Scaling

Axis can now be scaled by the user, as well as automatically from the data values. This allows for more flexibility in preparing consistent–looking plots.

Custom Labels

Plot titles, x– and y-axis labels, and legends labels can now be specified by the user as well as generated automatically. This will allow the DGUI to be used more for publication plots where custom labeling is important.
**Miscellaneous Other Improvements**

The ability to calculate the numerical first derivative of a time series was added.

The menu system was redone to provide compatibility with the Motif user interface and faster access to functions.

**Future Directions**

Currently the DGUI is used fairly frequently to examine both observed and computed data. It is powerful and stable enough to have become accepted as a normal tool for day-to-day use. Future development will probably be incremental in nature and largely driven by user requests.
Figure 6-1. Digital Filter

- Filtered Time series with long period pass filter
- Cutoff period: 30.2539 (hours)
Chapter 7

Data Assembly:
Time Series Data
Data Assembly: Time Series Data

The data assembly process for time series data was explained in the 1992 Annual Report. This section provides an update of the new data added to the database.

As of June 1994, the Delta Modeling Section has assembled and checked 12.2 million time series data points, an increase of about 50 percent from one year ago. Included in this number are 4.2 million regular time series (RTS) stage data points, 5.3 million RTS water quality points, 2.4 million RTS miscellaneous data such as flow, velocity, gate positions, air and water temperature, etc., and 358,000 grab-sample data points, collected on an irregular time basis.

The Delta Modeling Section expects several major sources of data to be copied to the database during the next year:

1. **Central District, DWR, Salinity, Stage, and Temperature.** DWR’s Central District has many years of 15-minute and daily salinity, stage, and temperature data. The Delta Modeling Section has only a small fraction of this, principally for 1988 calendar year. The Delta Modeling Section agreed to provide funds to the Central District so they can fully check and assemble their data for all years of record. This should add several million more data points.

2. **Information Systems and Services Office (ISSO), DWR.** The Water Information Management System (WIMS) database is maintained by ISSO. The Water Quality Module of this database was recently completed. During the coming year, new water quality data will be acquired from this source.

3. **Operations and Maintenance, DWR.** The Delta Modeling Section has started a significant investigation of data collections in the DWR’s Division of Operations and Maintenance. While this may not yield large amounts of data, the Delta Modeling Section expects that the data they have will not be readily available elsewhere and thus be quite valuable to our efforts. This should also be a good source of realtime data.

4. **U.S. Geological Survey.** The U.S. Geological Survey maintains a very large collection of data for both the San Francisco Bay and the Delta. The total collection is about 600 MB of compressed ASCII files. At this time we are unsure what fraction would pertain only to the Delta, but plan on getting a copy of all their Delta data within the next year. We already have some of their flow and stage data in the Delta.

5. **U.S. Corps of Engineers.** The U.S. Corps of Engineers is continuing their monitoring of surface and bottom velocity and salinity at three different locations in the Sacramento River. They have reworked the data and are ready to release it again. This would replace and extend the data we have already obtained from them.

6. **IESP Data Collection.** This is a database of the data collected by members of the Interagency Ecological Study Program.
15th Annual Progress Report

Chapter 8

Model Input System
The goal of a new input system is to make the models easier to use, decrease errors, and improve the model by allowing more precise and consistent time specifications. An easier-to-use model, with a decrease in input errors by users, should decrease the elapsed time from start to finish of a study using the numerical models. Improvements to the user interface are important to obtain a modeling system that can quickly produce reliable study results.

There are two categories of estuary model input: time-dependent and other.

Time-Dependent Input

Time-dependent input includes boundary stages, flows, water qualities, pumping rates, and timed gate operations. This time-dependent information will be input using the U.S. Army Corp of Engineers' Hydrologic Engineering Center Data Storage System (HECDSS), rather than reading from text files, for two reasons. First, HECDSS times are precise and consistent; it can specify timings down to the minute. Second, the times that things happen (changing flows, gates opening, etc.) are very clearly specified in both the input and the output, eliminating ambiguity and confusion.

To setup a model run, the user would input the time-varying data at the required locations into a HECDSS binary file. This input process could be done using a variety of methods. The most basic, or lowest level, would be to use the data utility editor DSSUTL and directly access the HECDSS file. This has the advantage of being the most flexible, but is cumbersome to use and is not generally the preferred method. Therefore an interface was developed to make the preparation of input data easier.

The core of the new time-varying input system interface is a text file with one input description per line. A description specifies the start and end dates and times, the time interval (hours, days, or months), the location, study name, parameter (stage, flow, etc.), repeat information (e.g. repeat every hour), and data value. This file is parsed with a program written in C and YACC, and the information is written to a HECDSS file. With the repeat information, one line could expand to many different time values in the HECDSS file, saving the user much effort.

The ASCII file itself could be created by hand, using any text editor, or with other interfaces. We developed an interface using GNU Emacs. This acts as an interactive form, allowing the user to enter information in an easy-to-use manner and trapping errors before they are written to the file. By using this interface, the user will be assured of a valid input file before the model run. Eventually, graphical input methods may be developed using the DGUI or similar package (Figure 8-1).

In general, at any location one could have multiple HECDSS pathnames (streams of input data), differentiated by parameter and study name. For instance, at the upstream boundary there might be multiple pathnames for Sacramento River flow, with different study names according to different flow rates. Other pathnames at the same locations would specify salt loading. There are potentially thousands of input locations and parameters for a model run: one pathname for each combination of location and parameter. Only a few of these pathnames are required for a model run: the boundary flows and salinities, and the downstream stage. Other pathnames are optional, but would typically be specified during a run: gate operations and important agricultural drainages and diversions.
Some method is needed to specify what pathnames to use at runtime, to specify which of multiple paths to use and to limit inquiries to HECDSS for paths that exist. The user will input a list of locations, parameters, study names, and time intervals to use. As it is running, the simulation model will consult this list to limit data acquisition from the HECDSS file to only those items in the list (Figure 8-2). This will also make it easy to change input from one study to the next, because all that is necessary would be a single change in study name. This list is part of the run control information and is inputted in the section described next.

**Other Input**

*Other input* consists of such things as geometry, run control, output control, and so on. Here the concept of orthogonality is important, that is, each logical input section should not have to be mixed in with other sections. For instance, when the user changes the output control, that should in no way affect the geometry specifications.

---

**Figure 8-1. Creating HECDSS Input**

**Figure 8-2. Selection of Time-Varying Data at Runtime**
Each logical section can be in one or more files and the user can repeat sections, with each subsequent section overlaying previous sections. This allows the use of basic files for most data, with overlay files changing only that data needed for the particular study.

Comments are permitted in the data input, which the input system ignores, and allows users to make notes for reference by others.

A basic table format of rows and columns is used for all data in this part of the input. Section headers tell the parser what kind of input to expect in the table (e.g., channel geometry data or run control information). Headers for each data field tell the input routine what data is in which field, so that the fields need not be in fixed order or columns. Then the data itself follows, in table format. Finally the table of data ends with a keyword.

Logical sections and field headers allow the users to specify a base run with a standard set of files, then specify a study run with only those changes needed for the study. For instance, if a study run changed only the width of one channel (i.e., for a dredging study), then the input for the study would consist of all the base run input, plus the one extra file with just a few lines specifying the changed channel. This will reduce both input errors and input setup time.

Currently the parsers for the time-varying data and the fixed data are working, and DSM2's Four-Point submodel is undergoing modification to use them. In the immediate future this work will continue and the Four-Point submodel will be connected to the new input system. After that, the BLTM submodel will be modified in a similar manner to use the new input system.

In the longer term, some of the input could be specified using the DGUI. For instance, it would be possible to change the dispersion coefficients in a group of channels to a fixed value by highlighting a region of channels and specifying the operation. This would allow a more intuitive way of entering input for the models.
15th Annual Progress Report

Chapter 9

Refinement of Carriage Water Routine
Refinement of Carriage Water Routine

Work continued by Delta Modeling staff to refine the carriage water routine used in DWRSIM's Minimum Delta Outflow (MDO) submodel. To date, a modeling approach superior to the current routine has not been developed. This chapter summarizes work that has been conducted over the past year to develop a refined model.

Statistical Analysis of Data

While under contract with DWR, R. Shumway and R. Azari of the University of California at Davis used time series analysis techniques to analyze historic flow and electrical conductivity data collected at several Delta locations (R.H. Shumway Consulting 1993). The consultants examined various approaches to selecting transformations and filters for linearizing flow concentration dynamics. Using 14-day moving averages, sampled weekly, they developed a linear transfer function model for predicting log proportional changes in concentration from past log proportional changes in concentrations and flows. It was noted that model uncertainty increases rapidly as the length of the forecast window increases. Therefore, the consultants concluded that the model is most applicable for making one- or two-week forecasts for given increases in flow or exports.

Transition Matrix Model Proposal

G. Bogle, a consultant for Water Engineering and Modeling, submitted a proposal to develop a simplified Delta hydrodynamic/water quality model to replace MDO (Water Engineering 1993). The key idea behind the use of the "transition matrix" model (TRANSAL) as a carriage water routine is that it offers the advantages of a more sophisticated numerical model (e.g. accuracy) along with much greater computational speed. Computational speed can be attained by saving and reusing simulation results from DWRDSM in matrix form. Because matrix development and TRANSAL calibration depends on a numerical Delta model, Delta Modeling staff determined that further consideration of this approach should be postponed until DWRSM2 is operational.

CCWD's Antecedent Outflow Model

Delta Modeling staff have studied the Antecedent Outflow (G) model developed by Contra Costa Water District (Denton 1993). This modeling approach is being used by staff to develop salinity-outflow relationships for several western Delta stations. The G model was applied to the analysis of EPA's proposed X2 standards (DWR 1994). It was observed to be quite sensitive to the weighting scheme selected to estimate model parameters. A project is currently being undertaken to compare the abilities of the G model and MDO in predicting salinity and required outflow to meet salinity standards at Rock Slough.
Refinement of Carriage Water Routine

Two-Straw Analysis

Delta Modeling staff undertook a study to develop a modified form of MDO while maintaining the basic net flow/Delta pool logic intact (DWR 1993). The main modification was to set western Delta salinity equal to Jersey Point salinity according to a salinity-outflow relationships developed by E. Winkler (DWR 1985). Possible extensions to this modeling approach might be to (1) incorporate the G model to predict Jersey Point salinity and (2) modify the MDO logic to incorporate tidal mixing and exchange (Denton and Hunt 1986).

References


Chapter 10

Two Part Per Thousand Isohaline Equation Analysis
The EPA's proposed estuarine standards are based on the 2 ppt bottom salinity isohaline (X2). This report shows that the method for determining X2 does not provide repeatable statistics and impact analysis.

The relevant X2 and flow data used to develop the daily and monthly X2 relationships used by the EPA for their standard was from Wim Kimmerer. The header and a sample of the data is shown in Table 10-1.

Table 10-1. Example of Kimmerer–Monismith Data

<table>
<thead>
<tr>
<th>Date</th>
<th>Interp X2</th>
<th>Log10 Qout X2</th>
<th>Best X2</th>
</tr>
</thead>
<tbody>
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<td>2/24/1968</td>
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Kimmerer–Monismith (K–M) filled in the gaps by first generating a linear relation between X2 and Log10 outflow using contiguous data between April 3, 1975, and December 31, 1977 (they did not specify the exact dates, only that they used the longest contiguous sequence in the 75–77 period). Using the resulting "Best X2" data, K–M determined a monthly X2–outflow relation.
Two Part Per Thousand Isohaline Equation Analysis

Analysis of the K-M X2 Model

An attempt was made to reproduce the daily equation results obtained by K–M. The Delta Modeling Section extracted the data for the period April 3, 1975 to December 31, 1977 (1003 days), created a column of the X2 data that was lagged one day from the daily X2, and regressed X2(t) on Log out(t) and X2(t−1). The resulting equation was:

\[ X2(t) = 8.48 + 0.953 \times X2(t−1) - 1.214 \times \log_{10} outflow \]

This compares well with the K–M equation:

\[ X2(t) = 10.16 + 0.945 \times X2(t−1) - 1.487 \times \log_{10} outflow \]

The difference is probably caused by using a slightly different data set window and are not considered to be significant. The residual standard error and \( R^2 \) of the equations are virtually identical.

Since the regression is defined in three-space, it cannot be easily shown graphically. Figure 10–1 shows the scatterplot of \( \log_{10} \) outflow versus \( X2(t) \) as well as the regression of \( X2(t) \) on \( \log_{10} \) outflow with the associated regression statistics. Also shown are the multiple regression statistics for \( X2(t) \) on \( X2(t−1) \) and \( \log_{10} \) outflow. The \( \log_{10} \) outflow explains 70 percent of the variance (\( R^2 = 0.70 \)), while the addition of \( X2(t−1) \) as an explanatory variable explains 99 percent of the variance (\( R^2 = 0.986 \)). This is possibly an inflated value, however, since \( \log_{10} \) outflow and \( X2(t−1) \) are highly correlated (Pearson's correlation coefficient = −0.84). The explanatory power provided by adding \( X2(t−1) \) is shown in Figure 10–3. There is a high correlation between \( X2 \) today and \( X2 \) yesterday.

Pursuing the \( X2(t) \) versus \( X2(t−1) \) correlation further, the entire filled-in record of \( X2 \) between October 1, 1967 and September 30, 1990 was plotted (Figure 10–4). The plot shows that \( X2 \) can travel up to 15 kilometers in one day, that there is no tendency to move upstream more or less than downstream in one day, and that daily movement of \( X2 \) is rather insensitive to position.

Regression residuals must meet four criteria before reliable inferences can be made:

1. The residuals must have a mean of zero. The mean for this model was calculated to be 0.00.
2. The residuals must be normally distributed. Figure 10–5 shows a histogram of the residuals. No hypothesis test was performed to prove normality, but the graphical evidence suggests the requirement is met.
3. The residuals must be independent. Figure 10–6 shows the residuals plotted in sequence and independence appears to exist.
4. Residuals versus explanatory variables should exhibit constant variance. Figures 10–7 and 10–8 show the residuals plotted against \( \log_{10} \) outflow (Figure 10–7), and \( X2(t−1) \) (Figure 10–8). There is some spreading with larger outflow and smaller \( X2(t−1) \), but it does not appear significant.

The regression provides an unbiased estimate of the physical trend within the range of the data, though collinearity of the explanatory variables should reduce the “goodness of fit” statistics somewhat.
Two Part Per Thousand Isohaline Equation Analysis

Regression of Log Outflow on X2(t) and X2(t−1)

There was some concern that solving the K–M X2 equation for outflow was an improper usage of the model because the error statistics for outflow estimates are undetermined, and the causal relation doesn’t exist physically. The modeling proceeded in the belief that since the R² is so high, there are no significant statistical pitfalls. After consulting with others, further investigation seemed prudent.

Figure 10-2 shows a scatterplot of X2(t) versus Log10 outflow, the regression of Log10 outflow on X2(t) with the model statistics, and the multiple regression statistics for Log10 outflow on X2(t) and X2(t−1). The addition of X2(t−1) as an explanatory variable in the multiple regression provides no additional prediction power over X2(t) alone. (The R² for Log10 outflow = f(X2(t)) is 0.7013, while the R² for Log10 outflow = f(X2(t), X2(t−1)) is 0.7015). Notwithstanding the incorrect conceptual model, predicting outflow from salinity is less reliable than predicting X2 from outflow and antecedent conditions.

1986–1989 X2 Equation

There is a long contiguous series of data between June 11, 1986 and March 26, 1989 (1018 days) in the K-M data. The same analysis was conducted on this data set as was conducted on the 1975–1977 data set. Comparing simple and multiple regression statistics on Figure 10-9, the correlation between X2(t) and Log10 outflow is relatively weak (R² = 0.35). However, when antecedent X2(t−1) is added, the R² improves to 0.96. Log10 outflow and X2(t−1) are again correlated (Pearson’s correlation coefficient = −0.59). It is unknown why the authors chose the 1975–77 data over the 1986–89 data and it is undetermined if the two models are the same statistically, though the water supply impacts are reduced using the 1986–89 equation (see below).

Figure 10-10 shows the outflow = f(X2(t), X2(t−1)) relation for the 1986–89 data. Again, no significant predictive power is provided by adding X2(t−1) as an explanatory variable (outflow = f(X2(t)), R² = 0.35; outflow = f(X2(t),X2(t−1)), R² = 0.38). In any case, impact analysis using this relation would be rather unreliable.

Impact Analysis Using Four Alternative X2–Outflow Relations

Four alternative methods are now available for determining the amount of additional releases required to meet the X2 standard on a given day. These are (1) regressions from the 1975–1977 sequence; (2) X2 on outflow solved for outflow; (3) outflow on X2; and (4) the same regressions for the 1986–1989 sequence. The four equations are now options in our X2 impact analysis routine. Table 10–2 shows the average yearly impact for the four equations.

<table>
<thead>
<tr>
<th>Table 10–2. Impact Of X2 Standard Using Alternative X2–Outflow Relations</th>
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<tr>
<td><strong>1975–1977 Sequence</strong></td>
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<tr>
<td>X2(t) = f (LOG10 OUTFLOW, X2 (-1)) (solve for outflow)</td>
</tr>
<tr>
<td>LOG10 OUTFLOW = f (X2 (t), X2 (t−1))</td>
</tr>
<tr>
<td><strong>1986–1989 Sequence</strong></td>
</tr>
<tr>
<td>X2(t) = f (LOG10 OUTFLOW,X2 (-1)) (solve for outflow)</td>
</tr>
<tr>
<td>LOG10 OUTFLOW = f (X2 (t), X2 (t−1))</td>
</tr>
</tbody>
</table>
Two Part Per Thousand Isohaline Equation Analysis

The X2 impact routine was run with a 14-day ramping period to bring X2 into compliance before February 14, the first day that a 14-day running average X2 must be in compliance.

In both sequences, the X2(t)=f(Log10 out, X2(t−1)) equations generate significantly larger impacts than the Log10 out=f(X2(t),X2(t−1)) equations. Examining the scatterplots (Figures 10-1, 10-2, 10-9, 10-10) gives some clues about this. The data shows that when X2 is above 80 kilometers, the corresponding outflows are more scattered. This can happen during the first days of higher outflows, when antecedent conditions are salty yet outflows are high. Minimizing the sum of the squared residuals about the X2 prediction is weighted by these anomalies toward more outflow. This is not the case for the estimate about outflow (Log10 outflow=f(X2(t),x2(t−1))).

The 1986–1989 sequence lowers overall impacts by about 8 percent (515 million acre-feet to 473 million acre-feet).

Comments

To analyze the impacts of the EPA proposal, it is necessary to determine the outflow required to meet the standard on any given day. Choosing to solve the physically meaningful X2 equation for outflow and loose statistical integrity or generating a causally backward relation between outflow and X2 can determine this. Both alternatives were investigated for two sections of the data. Some questions, concerns, and ideas for further study follow.

1. Why did the investigators choose to use the 1975–77 sequence rather than the 1986–89 sequence? The 1986–89 sequence is slightly longer, though the fit is not quite as good. It would be interesting to determine if the equations are the same statistically. If not, then there is a shift in the physics of the system between the two data sets. The questions is then which model is more appropriate to use?

2. The regression of Log10 outflow on X2 is somewhat unreliable. The R^2 for the 1975–77 sequence is 0.70 and the R^2 for the 1986–89 sequence is 0.38. These values are inflated by an undetermined amount by the co-variation of X2(t−1) and outflow. The residual standard error in the 1975–77 sequence is 0.218 and for the 1986–89 sequence is 0.278. At 12,000 cfs of delta outflow, this corresponds to a standard errors of 7,800 and 10,700 cfs, respectively. Perhaps more problematic is that predicting outflow from salinity cannot be justified physically.

3. Solving the X2(t)=f(Log10 outflow, X2(t−1)) relation for outflow is no less problematic. The modelers assumed that since the R^2 is so high, the variance characteristics of the estimate are not severely affected. Given the apparently large difference between the standard errors of the two approaches, this assumption is questionable.
FIGURE 10-1
CORRELATION BETWEEN X2 AND REVISED DAYFLOW OUTFLOW

\[ X_2 = f(\text{DELTA OUTFLOW}) \quad (4-3-75 \rightarrow 12-31-77) \]

**FIGURE 10-2**
DELTA OUTFLOW = f(X2) \quad (4-3-75 \rightarrow 12-31-77)
FIGURE 10-3

CORRELATION BETWEEN X2(t) AND X2(t-1)
(Kimmerer-Monismith Equation data; 4-3-75 through 12-31-77)

RESIDUAL STANDARD ERROR = 1.332182
R-SQUARE = 0.9855
DEGREES OF FREEDOM = 1002

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<th>T STAT</th>
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<td>LOG OUTFLOW</td>
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X2 TODAY (KM)

X2 YESTERDAY (KM)
FIGURE 10-4
CORRELATION BETWEEN X2(t) AND X2(t-1)
(Kimmerer-Monismith Equation data; 10-1-67 through 9-30-90)

- Shows the distance X2 can travel in one day
- Shows no bias toward up or downstream movement
- Shows that daily movement is insensitive to position
FIGURE 10-5
HISTOGRAM OF RESIDUALS

\( X_2(t) = f(\text{Delta Outflow}, X_2(t-1)) \quad 4-3-75 \rightarrow 12-31-77 \)
FIGURE 10-6

RESIDUAL ANALYSIS PLOTS: Kimmerer-Monismith Data

\[ X_2(t) = f(Delta \ Outflow, X_2(t-1)) \ 4-3-75 \rightarrow 12-31-77 \]

FIGURE 10-7

LOG OUTFLOW vs RESIDUALS

FIGURE 10-8

\[ X_2(t-1) \] vs RESIDUALS
FIGURE 10-9
CORRELATION BETWEEN X2 AND REVISED DAYFLOW OUTFLOW
\[ X2 = f(\Delta \text{OUTFLOW}) \ (6-11-86 \rightarrow 3-26-89) \]

\[
\begin{align*}
X2(t) &= I (\Delta \text{OUTFLOW}) \\
\text{RESIDUAL STANDARD ERROR} &= 0.352278 \\
\text{R-SQUARE} &= 0.396277 \\
\text{DEGREES OF FREEDOM} &= 1017 \\
\text{COEF} &\begin{cases}
\text{STD ERR} & \text{T STAT} \\
130.1353 & 1.883558 \\
-12.34768 & -12.04806
\end{cases}
\end{align*}
\]

\[
\begin{align*}
X2(t) &= I (\Delta \text{OUTFLOW}, X2(t-1)) \\
\text{RESIDUAL STANDARD ERROR} &= 0.352278 \\
\text{R-SQUARE} &= 0.396277 \\
\text{DEGREES OF FREEDOM} &= 1017 \\
\text{COEF} &\begin{cases}
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-0.0704279 & \text{X2(1)} \\
0.0431418 & 0.00685552 \\
0.0000204 & 0.0000204
\end{cases}
\end{align*}
\]

FIGURE 10-10
DELTA OUTFLOW = f(X2) \ (6-11-86 \rightarrow 3-26-89)

\[
\begin{align*}
\text{DELTA OUTFLOW} &= f(X2(t)) \\
\text{RESIDUAL STANDARD ERROR} &= 0.295387 \\
\text{R-SQUARE} &= 0.396277 \\
\text{DEGREES OF FREEDOM} &= 1017 \\
\text{COEF} &\begin{cases}
\text{STD ERR} & \text{T STAT} \\
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-0.0283881 & \text{X2(1)} \\
0.0431418 & 0.00685552 \\
0.0000204 & 0.0000204
\end{cases}
\end{align*}
\]

\[
\begin{align*}
\text{DELTA OUTFLOW} &= f(X2(t), X2(t-1)) \\
\text{RESIDUAL STANDARD ERROR} &= 0.295387 \\
\text{R-SQUARE} &= 0.396277 \\
\text{DEGREES OF FREEDOM} &= 1017 \\
\text{COEF} &\begin{cases}
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0.0431418 & 0.00685552 \\
0.0000204 & 0.0000204
\end{cases}
\end{align*}
\]