PARAMETER IDENTIFICATION IN ESTUARINE MODELING

Wen-Sen Chu[1] and William W-G. Yeh[2]

INTRODUCTION

Parameter Identification (PI) algorithm is an optimization procedure that systematically searches the parameters embedded in a mathematical model. These parameters are not measurable from a physical point of view. The optimization is based on the minimization of a selected norm of the differences between the solution of the mathematical model and scattered observations collected from the system.

Parameter identification (or inverse problem) has been studied in groundwater systems extensively for the past decade (15), and it has also drawn many researchers in the fields of open-channel flow and estuarine modeling since 1972 (1,2,9,17). All the past estuarine PI works in the literature are confined to the one-dimensional case, and hydrodynamics and transport equations are treated separately.

This study deals with PI in a two-dimensional vertically-averaged estuarine salinity model. The salinity transport equation is coupled with the hydrodynamics equations. The coupled relationship introduces extra density terms in the hydrodynamics equations, which must be solved simultaneously with the transport equation.

One of the most difficult problems in PI is the collection of needed observations from the system which is being modeled. With limited exception, the currently available data from the prototype estuaries are not adequate for the purposes of developing a PI algorithm. This is usually critical in quantity (the number of stations and/or the period of time) and in quality (noise of data). However, if an operational hydraulic model is available, the data could then be obtained economically and accurately under an ideally controlled environment. The large amount of data that can be collected from a hydraulic model of an estuary will provide a sufficient number of observations and the required initial and boundary conditions for the development of a PI algorithm. The use of the estuary hydraulic model could provide a better source of prototype data than would be available from the real estuary. It will be much easier to distinguish between the inadequacy of the mathematics and the inadequacy of our understanding of the prototype. Thus, it will give us an idea of how well we could expect to mathematically model the real estuary if we had an unlimited amount of prototype data. Additionally, when these types of data are used in PI, parameters can be optimally identified and the mathematical model can then be used conjunctively with the hydraulic model for prototype applications, provided that the mathematical model is consistently formulated. How well a hydraulic model simulates the prototype estuary is not considered in this study.

[1]Assistant Professor, Department of Environmental Resources Engineering, Humboldt State University, Arcata, California 95521. (Formerly, Graduate Student, School of Engineering and Applied Science, University of California, Los Angeles, California 90024).

[2]Professor, School of Engineering and Applied Science, University of California, Los Angeles, California 90024.

A tidally averaged approach is adopted to furnish the mathematical model solutions for the purpose of PI. This particular approach solves the dynamic steady-state conditions of the variables as represented by their time-averaged values. The mathematical model of this type is a boundary-value problem, and it is solved by an implicit-explicit iterative scheme (3,4). The rationale of using a tidally averaged model in PI is based upon the assumption that the parameters to be identified are time-invariant, i.e., the parameters have the same values in the transient and dynamic steady-state conditions.

The Error Function Method (1,4) is used with minimax criterion in the optimization. Error function is linearized so that when it is used with the minimax criterion, the optimization problem can be transformed into a Linear Programming (LP) problem.

TIDALLY AVERAGED APPROACH

In order to formulate the two-dimensional vertically averaged mathematical model (See Figure 1) that approximates the prototype conditions as represented by the fixed-bed hydraulic model, the following transient equations are used (11,12):

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial \xi}{\partial x} + g\langle i\rangle_x + g\frac{u(u^2+v^2)^{1/2}}{C^2 H} = 0 \qquad (1)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial \xi}{\partial y} + g\langle i\rangle_y + g\frac{v(u^2+v^2)^{1/2}}{C^2 H} = 0 \qquad (2)$$

$$\frac{\partial \xi}{\partial t} + \frac{\partial (Hu)}{\partial x} + \frac{\partial (Hv)}{\partial y} = 0 \qquad (3)$$

$$\frac{\partial (Hs)}{\partial t} + \frac{\partial (Hus)}{\partial x} + \frac{\partial (Hvs)}{\partial y} - \frac{\partial}{\partial x}\left(HD_x\frac{\partial s}{\partial x}\right) - \frac{\partial}{\partial y}\left(HD_y\frac{\partial s}{\partial y}\right) = 0, \qquad (4)$$

in which u, v are the velocities in x, y directions: ξ is a tidal elevation with respect to mean sea level h; $H = \xi + h$; s is salinity; C is the Chezy's coefficient; D_x and D_y are the dispersion coefficients; g is gravitational acceleration; and $\langle i\rangle_x$ and $\langle i\rangle_y$ are the density slope terms induced by salinity. The density terms can be represented in English unit system by (12, 14):

$$\langle i\rangle_x = \frac{1.94 \times 10^{-3}}{1.94 + 1.94 \times 10^{-3}\sigma_t}\frac{\partial \sigma_t}{\partial x} \cdot \frac{H}{2} \qquad (5)$$

$$\langle i\rangle_y = \frac{1.94 \times 10^{-3}}{1.94 + 1.94 \times 10^{-3}\sigma_t}\frac{\partial \sigma_t}{\partial y} \cdot \frac{H}{2}, \qquad (6)$$

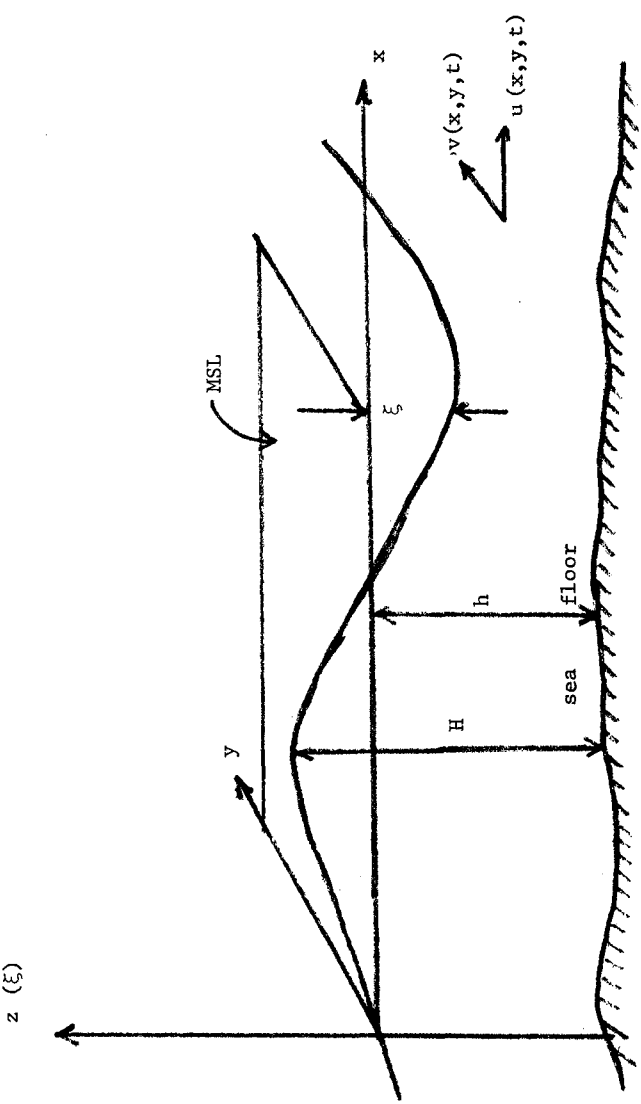

Fig. 1.- Two-Dimensional Estuarine Coordinate System

in which σ_t is the oceanographical sigma-tee function whose values depend upon salinity and temperature.

Coriolis force and wind stress are not included in Eqs. (1) and (2) to conform with the hydraulic model conditions.

For the purpose of this study, the following equation is used for Chezy's C:

$$C = \sqrt{2g/f} \quad , \tag{7}$$

in which f is the Darcy's roughness coefficient, which can be assumed to be time-invariant (5).

Using previous findings (8,10,11), the dispersion coefficients can be written as:

$$D_x = DCX \cdot H \cdot |u| \cdot g^{1/2} \cdot C^{-1} \tag{8}$$

$$D_y = DCY \cdot H \cdot |v| \cdot g^{1/2} \cdot C^{-1} \quad , \tag{9}$$

in which DCX and DCY are assumed to be constants representing the characteristics of the particular estuary; and $|u|$, $|v|$ are the velocities in x and y directions.

When the boundary conditions of the transient model can be assumed to be periodic, all transient variables will reach a dynamic steady-state after a long period of time. These dynamic steady-state variables are constant over time when they are averaged over the period. They are defined as tidally averaged variables when the period used is a tidal cycle.

When Eqs. (1) to (9) are tidally averaged, they can be written as (3,4):

$$U \frac{\partial U}{\partial x} + V \frac{\partial U}{\partial y} + g \frac{\partial \hat{\xi}}{\partial x} + g\langle \bar{i} \rangle_x + g \frac{U(U^2+V^2)^{1/2}}{C^2 \bar{H}} = 0 \tag{10}$$

$$U \frac{\partial V}{\partial x} + V \frac{\partial V}{\partial y} + g \frac{\partial \hat{\xi}}{\partial y} + g\langle \bar{i} \rangle_y + g \frac{V(U^2+V^2)^{1/2}}{C^2 \bar{H}} = 0 \tag{11}$$

$$\frac{\partial (\bar{H}U)}{\partial x} + \frac{\partial (\bar{H}V)}{\partial y} = 0 \tag{12}$$

$$\frac{\partial}{\partial x}(\bar{H}US) + \frac{\partial}{\partial y}(\bar{H}VS) - \frac{\partial}{\partial x}\left(\bar{H}\bar{D}_x \frac{\partial S}{\partial x}\right) - \frac{\partial}{\partial y}\left(\bar{H}\bar{D}_y \frac{\partial S}{\partial y}\right) = 0, \tag{13}$$

and,

$$\langle \bar{i} \rangle_x = \frac{1.94 \times 10^{-3}}{1.94 + 1.94 \times 10^{-3}\bar{\sigma}_t} \frac{\partial}{\partial x} \bar{\sigma}_t \cdot \frac{\bar{H}}{2} \tag{14}$$

$$\overline{\langle i \rangle}_y = \frac{1.94\times10^{-3}}{1.94+1.94\times10^{-3}\bar{\sigma}_t} \frac{\partial}{\partial y}\bar{\sigma}_t \cdot \frac{\bar{H}}{2} \tag{15}$$

$$C = \sqrt{2\,g/f} \tag{16}$$

$$\bar{D}_x = DCX \cdot \bar{H} \cdot |U| \cdot g^{1/2} \cdot C^{-1} \tag{17}$$

$$\bar{D}_y = DCY \cdot \bar{H} \cdot |V| \cdot g^{1/2} \cdot C^{-1} \tag{18}$$

in which U, V, $\hat{\xi}$, S, $\langle\bar{i}\rangle$ are the tidally averaged values of u, v, ξ, s, $\langle i \rangle$; and $\bar{H}$ is equal to $h + \hat{\xi}$. The detailed mathematics of this approach are given by Chu and Yeh (3) and Chu (4) which will not be included here. The key assumption for the averaging process is that all the transient variables have small amplitudes in time. The concept of the averaging process is similar to the one that was used in vertical averaging by Leendentse (11).

The parameters to be identified in the above tidally averaged model are the Darcy's roughness coefficient f, and the two dispersion constants DCX and DCY. The parameters, by the previous assumptions, will have the same values in both the transient and the tidally averaged models.

The distinct advantage of using the tidally averaged approach, despite the above-mentioned assumptions, is the saving of computing cost. If a transient model is used for PI, long term integration is likely to be required to generate solutions that are commensurate with observations. Since most of the identification schemes require an iterative search process, such long term integration can easily discourage the modelers' desire for PI, let alone their concerns over the accumulated errors generated by such extended runs.

Equations (10) through (18) are solved by an implicit-explicit, alternating direction, iterative finite difference scheme developed by Chu and Yeh (3). The method is conceptually similar to the multi-operational, implicit-explicit scheme by Leendentse for the transient problem (11). Instead of integrating in time, an acceleration parameter is used for each iteration. The convergence of the proposed scheme is fairly rapid for hydrodynamics and slow for salinity transport. Since its development, the algorithm has been numerically verified through a series of test problems (3,4). These test problems include various initial and boundary conditions. The results showed that the numerical model is applicable to any two-dimensional estuarine problem. Detailed computational aspects of the scheme are given in Chu and Yeh (3) and Chu (4) and they will not be covered here.

PARAMETER IDENTIFICATION ALGORITHM

The selected norm for this study is the minimax criterion, which minimizes the absolute value of the maximum error among all observation stations in the domain. Mathematically, it is to

$$\min_{\vec{D}} \max_{1\le i\le M} \left| \sum_{k=1}^{L} W_{ik}\, \varepsilon_{ik} \right|, \tag{19}$$

in which $\vec{D}$ represents the parameter vector in the model; and ε_{ik} is the error at station i of the kth variable which is collected as observation. Equation (19) implies that all k variables are observed at the same stations, i = 1,...,M. W_{ik} in Equation (19) is a weighting factor. These weighting factors are necessary to reflect widely differing numerical values and units.

If tidal elevations and salinities are available at stations i = 1,...M, we can rewrite Equation (19) as:

$$\min_{\vec{D}} \max_{1\le i\le M} \left\{ |W_{i1} \cdot \varepsilon_i| + |W_{i2}\, \eta_i| \right\} \tag{20}$$

$$\varepsilon_i = \hat{\xi}_i - \hat{\xi}_i^* \tag{21}$$

$$\eta_i = S_i - S_i^*, \tag{22}$$

in which $\hat{\xi}^*$ and S* are the observations.

In this study, ε_i and η_i are assumed to be functions of the parameters only; i.e., it is assumed that the differences between the model solutions and the observations are due to incorrect quantification of the model parameters. Given this assumption, error function can be written in vector notation as:

$$\vec{\varepsilon}(\vec{D}) = (\varepsilon_1(\vec{D}),\ldots,\varepsilon_M(\vec{D})). \tag{23}$$

$$\vec{\eta}(\vec{D}) = (\eta_1(\vec{D}),\ldots,\eta_M(\vec{D})) \tag{24}$$

The parameter vector $\vec{D}$ can be written as $\vec{D} = (\vec{f},DCX,DCY)$, in which DCX and DCY are assumed to be pure constants.

By Taylor's theorem, Equations (23) and (24) can be expanded at some initially estimated parameters $\vec{D}^o$ as

$$\vec{\varepsilon}^1(\vec{D}^1) = \vec{\varepsilon}^o(\vec{D}^o) + J(\vec{\varepsilon}^o,\vec{D}^o)(\vec{D}^1-\vec{D}^o) + H.O.T., \tag{25}$$

$$\vec{\eta}^1(\vec{D}^1) = \vec{\eta}^o(\vec{D}^o) + J(\vec{\eta}^o,\vec{D}^o)(\vec{D}^1-\vec{D}^o) + H.O.T., \tag{26}$$

in which the superscript 1 represents the new estimates; H.O.T. are the higher order terms; and J (,) is the Jacobian matrix.

When H.O.T. are dropped, Equations (25) and (26) become linear with the Jacobian being approximated by finite difference. The finite difference version of the Jacobian is referred to by Becker and Yeh (1) as the Influence Coefficient Matrix.

After transforming Equation (20) to a linear objective function, the optimization problem becomes a linear programming problem. Physical constraints representing parameter lower and upper bounds can be imposed for optimization to ensure realistic solutions.

The solutions of the LP will provide the minimized error and a set of new parameters $\tilde{D}^1$. These new parameters then become the initial estimates for the next iteration. The algorithm continues until the convergence criteria are satisfied. Two types of convergence criteria are proposed in this method; they are 1) stop when $|J^K| < \delta_1$, and 2) stop when $|J^{K+1} - J^K| < \delta_2$, in which J^K is the objective value of the LP solution at the Kth iteration, and δ_1 and δ_2 are two arbitrarily selected small constants.

The most important merit of the proposed method is that it is independent of the mathematical model, and it can be implemented and solved efficiently in any modern computer facility where packaged routines are available for linear programming problems.

NUMERICAL EXAMPLE

Suisun Bay in California was selected for this study (see Figure 2). Tidal elevations and salinities were obtained in the Suisun Bay portion of the San Francisco Bay - Delta Hydraulic Model in Sausalito, California (13). The finite difference schematization of Suisun Bay is shown along with the installed observation stations in Figure 3. Bathymetric schematization was obtained according the actual blueprints for the construction of the model (13).

The first PI attempt assumes that all the unknown parameters are constant valued in the domain. The physical bounds set for the parameters are: 1) $0.01 \leq f \leq 0.1$ (which corresponds to the Chezy's C values between 25 ft $^{1/2}$/sec and 80 ft $^{1/2}$/sec), 2) $1000 \leq DCX \leq 7000$, and 3) $1000 \leq DCY \leq 5000$. These physical bounds are determined not only by the physical laws but also by computational experience through sensitivity analyses of the parameter values. For example, through various test runs, it was determined that the dispersion constants DCX and DCY would have to enlarged in order to "reflect" the boundary salinities toward the interior of the domain.

The PI algorithm started with a set of initial estimates of: 1) $f^o = 0.05$, 2) $DCX^o = 3500$, and 3) $DCY^o = 3000$. The computed solutions using the estimated parameters are compared with the observations in Table 1. The convergence property of this run is shown in Table 2.

The second attempt of the PI is much more refined. The roughness coefficient is assumed to be spatially distributed in Suisun Bay. The dispersion constants remain constant valued because of their insensitivity in the model simulations.

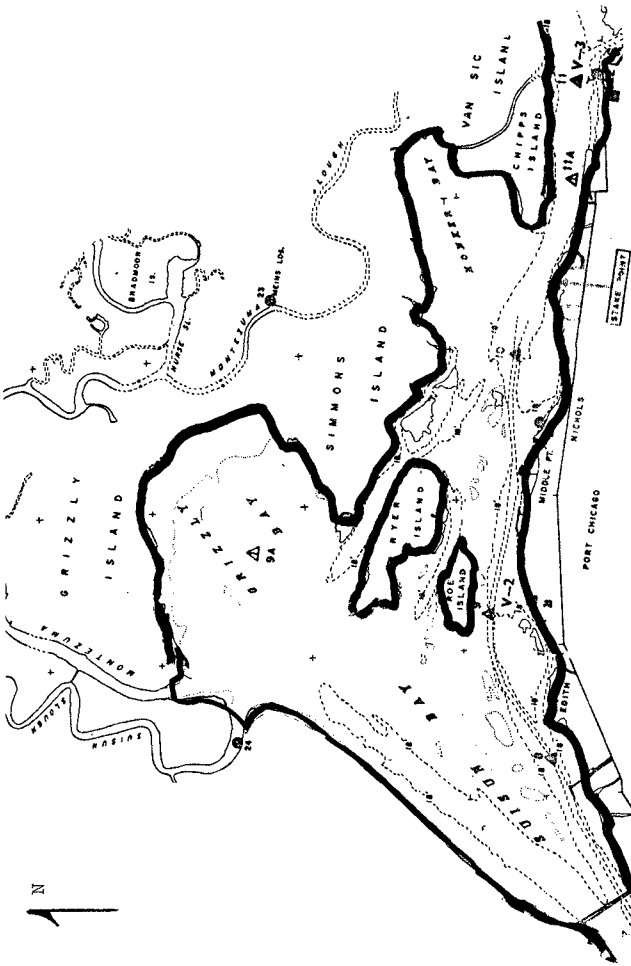

Fig 2. Map of Suisun Bay. (Courtesy of U.S. Army Corps of Engineers, San Francisco District.)

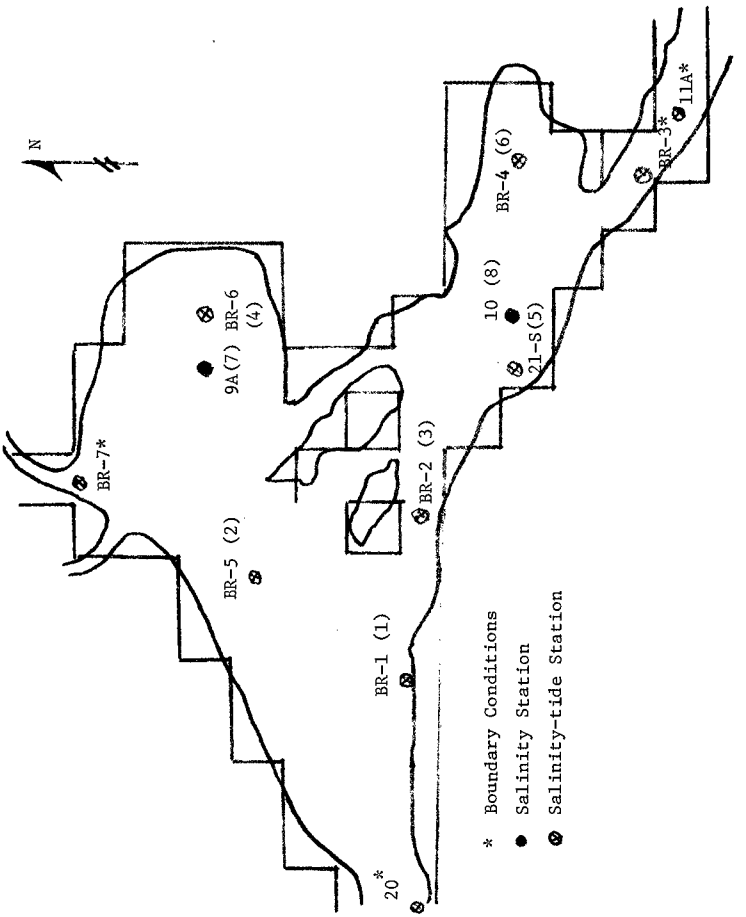

Fig. 3 Finite Difference Schematization and Observation Stations in Suisun Bay

TABLE I.- Summary of Computational Results
(Lumped Parameter Case[4])

Station No.	Obs. $\hat{\xi}$[1]	Comp. $\hat{\xi}$[1]	Obs. S[3]	Comp. S[3]	ε^2	η^2
1	0.27	0.17	11.09	9.29		
2	0.32	0.19	7.99	6.92		
3	0.23	0.20	8.45	6.40		
4	0.41	0.21	5.40	7.05	0.19	1.74
5	0.29	0.25	5.0	3.56		
6	0.40	0.27	3.2	3.15		

1 $\hat{\xi}$ is net tide in ft.

2 Minimized maximum errors

3 S is tidally averaged salinity in ppt

4 Optimal parameters: $f = 0.06$ ($C = 32$ ft $^{1/2}$/sec)
DCX = 7000.
DCY = 5000.

Boundary conditions used for parameter identification (calibration):

Ocean boundary: $\hat{\xi} = 0.12$ ft
S = 13.71 ppt

Fresh Water Inflows: U (Sacramento River) = -0.34 ft/sec
S (Sacramento River) = 2.5 ppt
V (Montezuma Slough) = -0.1 ft/sec
S (Montezuma Slough) = 5.68 ppt

TABLE 2. - Summary of Successive Approximations
(Lumped Parameter Case)

Iteration	f	DCX ($\times 10^{-3}$)	DCY ($\times 10^{-3}$)	J
0	0.05	3.5	3.0	4.85
1	0.07	7.0	4.5	2.00
2	0.10	5.3	5.0	1.95
3	0.06	7.0	5.0	1.94

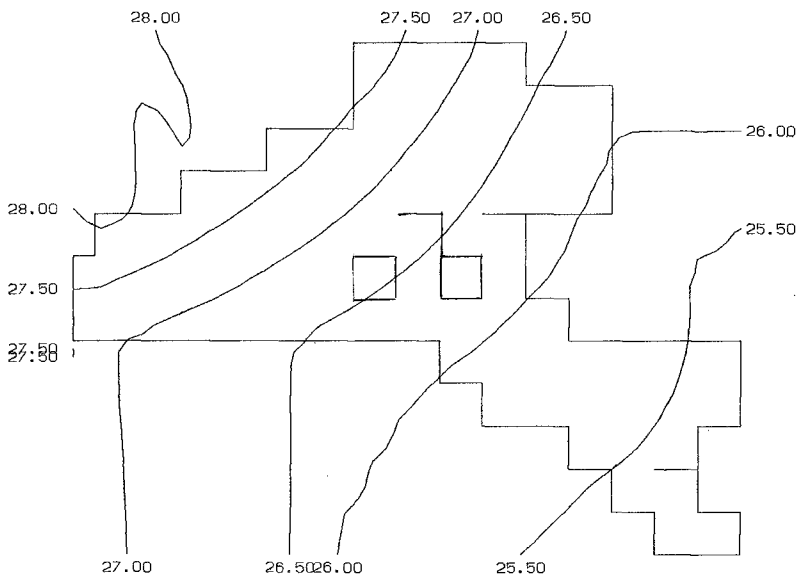

Figure 4. Spatial Distribution of Chezy's C.

Given the above proposed distributed parameter assumption, the PI algorithm would have to identify roughness coefficient at all nodal points. This is such a large task that it is almost impossible to accomplish with the fastest computer available. Furthermore, parameter values between the nodes show discontinuities which do not have any physical meaning. This difficulty has been resolved with the help of the finite element concept by Yeh and Yoon (16) and Yoon and Yeh (18) in PI problems of groundwater flow.

It appears that roughness parameter space in Suisun Bay can be adequately represented by the four corner nodes with bilinear basis functions (4,16). Mathematically, it is

$$f(x,y) = \sum_{i=1}^{4} f_i \, \phi_i(x,y), \tag{27}$$

in which f_i's are the corner nodal values; and ϕ_i's are the bilinear basis functions. With Equation (27), the parameter values in any grid point of Suisun Bay could be calculated given nodal values of f_i's. The algorithm is then to identify the four nodal values (f_i's) instead of searching through all the grid points.

The physical bounds and the initial estimates for the parameters remained the same in this run. The algorithm converged in eight iterations. The optimally estimated roughness parameters vary from 0.07 to 0.1, which correspond to the Chezy's values of 25 ft $^{1/2}$/sec to 30 ft $^{1/2}$/sec. The distributed values as estimated by the PI algorithm are shown in Figure 4. The optimal dispersion constants converged to be at 7000 and 1000. The computed solutions using the optimal parameters are compared with the observations in Table 3. The convergence property of this run is shown in Table 4.

To validate the results of calibration, the optimized parameters were used as input data along with a different set of boundary conditions, which were consistent with the experimental set up, in the tidally averaged numerical model to produce solutions. These solutions were compared with the experimental data taken from the San Francisco Bay-Delta Hydraulic Model. The boundary conditions (fresh water inflow and tide) used in the verification and the corresponding experiment were different from the boundary conditions used in the calibration.

Since there is no significant difference in results between the lumped parameter and distributed parameter approach (see Tables 1 and 3), the lumped parameters were used for verification. The verification run started with a set of initial conditions (identical to the ones used in calibration), boundary conditions, and the optimized parameters which are: 1) f = 0.06 , 2) DCX = 7000, and 3) DCY = 5000 (see Table 1). The verification results and the boundary conditions used are presented in Table 5.

DISCUSSION AND CONCLUSION

Although the tidally averaged numerical model can save a signifi-

Table 3. Summary of Computational Results
(Distributed Parameter Case[4])

Station	Obs.$\hat{\xi}$[1]	Comp.$\hat{\xi}$[1]	Obs.S[3]	Comp.S[3]	ε[2]	η[2]
1	0.27	0.17	11.09	9.71		
2	0.32	0.19	7.99	7.37		
3	0.23	0.20	8.45	6.95		
4	0.41	0.23	5.40	7.35	0.18	1.45
5	0.29	0.27	5.00	3.86		
6	0.40	0.30	3.20	3.33		
7	-	-	5.49	6.33		
8	-	-	4.39	3.66		

1 $\hat{\xi}$ is net tide in ft.

2 Minimized maximum errors

3 S is tidally averaged salinity in ppt.

4 Optimum parameters:

f in nodal values $\begin{cases} f_1 = 0.07 & C_1 = 30 \text{ ft}^{1/2}/\text{sec} \\ f_2 = 0.10 & C_2 = 25 \text{ ft}^{1/2}/\text{sec} \\ f_3 = 0.10 & C_3 = 25 \text{ ft}^{1/2}/\text{sec} \\ f_4 = 0.10 & C_4 = 25 \text{ ft}^{1/2}/\text{sec} \end{cases}$

DCX = 7000.

DCY = 1000.

TABLE 4. - Summary of Successive Approximation

(Distributed Parameter Case)

Iteration	f_1	f_2	f_3	f_4	DCX ($\times 10^{-3}$)	DCY ($\times 10^{-3}$)	J
0	0.05	0.05	0.05	0.05	3.5	3.0	4.85
1	0.05	0.01	0.10	0.08	7.0	5.0	2.02
2	0.06	0.10	0.10	0.10	7.0	5.0	1.73
3	0.07	0.01	0.10	0.01	7.0	5.0	1.90
4	0.07	0.10	0.10	0.10	7.0	1.0	1.52

Table 5. Results of Steady-State Model Verification

Station No.	Obs. $\hat{\xi}$[1]	Comp. $\hat{\xi}$[1]	Obs. S[2]	Comp. S[2]
1	0.09	0.04	16.89	14.81
2	0.06	0.04	13.95	12.41
3	0.10	0.06	14.81	11.86
4	0.26	0.08	11.77	10.62
5	0.15	0.11	11.60	9.28
6	0.28	0.13	9.39	8.99

Boundary conditions used for verification:

Ocean boundary: $\hat{\xi}$ = - 0.01 ft

S = 19.31 ppt

Fresh water inflows: U (Sacramento River) = - 0.33 ft/sec

S (Sacramento River) = 8.34 ppt

V (Montezuma Slough) = - 0.01 ft/sec

S (Montezuma Slough) = 12.19 ppt

1 net tide in feet

2 tidally average salinity in ppt.

cant amount of computing time in PI, the convergence of the solution scheme is still slow; especially when the transport equation is coupled with the hydrodynamics. The solutions of hydrodynamics alone will usually converge within 200 iterations with variable acceleration parameters (3,4). Nevertheless, when salinity transport equation is calculated with hydrodynamics, the algorithm will typically require 400 iterations to converge. The convergence of salinity values depends on the corresponding hydrodynamics. When the magnitudes of hydrodynamics (velocities and tides) are small, the convergence property of salinities is also influenced by the initial conditions of salinity (3,4). This particular computational problem is solved by a series of semi-heuristic rules that are determined from the computational experience (4).

When the transient numerical model is simulated, the outputs of the model are generally insensitive to different values of dispersion constants (DCX, DCY). In one particular simulation for example, two sets of dispersion constants which differed in value as great as 100 times produced only 1 to 5% changes in salinities in ten tidal cycles. Nevertheless, when tidally averaged numerical model is simulated with the true boundary values collected from the hydraulic model, it was found that the dispersion constants would have to be enlarged in order to "reflect" the ocean boundary salinities toward the interior of the domain. One of the conceivable reasons for this phenomenon is the strong net outflow from the delta to the ocean. This limited increase of the internal salinity values in the domain in tidally averaged numerical model is due to the inherent nature of the boundary value problems (Eqs. 10 to 14). Other factors that may cause the inflation of the dispersion constants include: the finite difference schematization, the vertical averaging, the tidal averaging, and the various model approximations.

The proposed PI algorithm is independent of the numerical model by virtue of the error function approach. By the definition of error function and the problem formulations, the identification algorithm can be programmed separately from the numerical model. In other words, the method can be easily implemented with any numerical model for PI purposes, provided that enough data are available.

The calibration and verification of the tidally averaged numerical model have been successfully performed. In both attempts, the maximum deviations between the model results and field observations came from the particular station in Grizzly Bay. In the schematization of the entire study area, the inflow from Suisun Slough which is next to Montezuma Slough was ignored. The performance of the mathematical model depends not only on its parameter values, but also on the schematizations. Other important factors that could contribute the discrepancies include noises in observations and errors in data processing of boundary conditions and observations (4).

In each iteration of PI, the numerical model has to be solved once for each parameter in order to generate the influence coefficient matrix. In the lumped parameter approach, (three constant parameters for the entire domain), it took three iterations for the PI scheme to converge. (The numerical models had been solved by $3 \times 3 + 3 = 12$ times.) This lumped parameter PI case used 20 minutes of IBM 360/91 computing time at a cost of $150 dollars.

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