Validation of DSM2 QUAL for Simulation of Various Cations and Anions

Prepared for: Metropolitan Water District of Southern California

By: MWH

Final Report

June 2012

Table of Contents

Tables

Figures

Attachments

List of Abbreviations and Acronyms

CDEC	California Data Exchange Center
Delta	Sacramento-San Joaquin Delta
DO	dissolved oxygen
DOC	dissolved organic carbon
DWR	California Department of Water Resources
EC	electrical conductivity
IEP	Interagency Ecological Program
NRMSE	normalized root mean square error
meq/L	milliequivalent per liter
RMSE	root mean square error
TDS	total dissolved solids
µS/cm	microsiemens per centimeter

1.0 Introduction

The Delta Simulation Model II (DSM2) is a one-dimensional mathematical model for simulating Sacramento-San Joaquin Delta hydrodynamics, water quality, and particle tracking. Historically, simulated Delta hydrodynamics and water quality conditions were validated through comparison with available hydrodynamics and electrical conductivity (EC) data in the Delta. The validation process resulted in an overall good fit with the field data for stage, flow, and water quality (Nader-Tehrani, 2001; Thein, 2006). Validation of the PTM module has not been completed due to limited data regarding the transport and fate of individual particle data.

There are concerns about DSM2's ability to simulate other salinity constituents using the existing model. DSM2 was calibrated using EC as the target salinity. Concerns have been raised about using EC for calibrating dispersion factors due to its failure to behave as a truly conservative indicator of salinity. As salinity and ionic concentration increase, EC increases. At higher salinity concentrations, ion mobility is depressed and ability to transmit electrical current is impaired. As a result, EC increasingly underestimates true salinity at higher concentrations, a trend manifest in a nonlinear relationship between EC and any conservative constituent (Suits, 2002). Based on the concerns mentioned above, it is necessary that the DSM2 model be validated for water quality constituents other than EC to enhance the reliability of the model.

1.1 Study Purpose

The purpose of this study is to evaluate the effectiveness of the DSM2 model in simulating various anions (chloride, bromide, sulfate, and bicarbonate) and cations (sodium, magnesium, and calcium) at various locations in the Delta. This report documents this evaluation effort.

1.2 Report Organization

Chapter 1 provides a brief overview of the model and the purpose of this report. Chapter 2 provides an overview of the DSM2 model, the DSM 2 QUAL module that simulates Delta water quality, and the historical DSM2 simulation model maintained by DWR. Chapter 3 describes the methodology and data used to complete this validation evaluation effort. Chapter 4 describes the model validation results for EC and other cations and anions. Chapter 5 presents the conclusions of the study and recommendations. Chapter 6 presents the reference cited in this document.

2.0 Background

This chapter provides an overview of the DSM2 model, the DSM 2 QUAL module that simulates Delta water quality, and the historical DSM2 simulation model maintained by DWR.

2.1 DSM2 Model General Overview

DSM2 can calculate stages, flows, velocities, transport of individual particles, and mass transport processes for conservative and non-conservative constituents, including salts, water temperature, dissolved oxygen (DO), and dissolved organic carbon (DOC). DSM2 includes three Modules: HYDRO (hydrodynamics), QUAL (water quality), and PTM (particle tracking). The HYDRO module is a tool to study the complex tidal hydraulic system in the Delta. The QUAL module is a one-dimensional transport model that predicts the fate of various water quality constituents. The PTM module simulates the transport and fate of individual particles traveling throughout the Delta. The QUAL module is the focus of this study and is discussed further below.

2.2 DSM2-QUAL

DSM2-QUAL is based on a one-dimensional advection-dispersion equation to simulate the transport of water quality constituents in open channels. The flow field computed by HYDRO provides needed information for the advection part of the transport process. Transport via dispersion is computed based on the input dispersion coefficient and the concentration gradient calculated during simulation.

The transport simulation of any water quality constituent in DSM2 requires input of the dispersion coefficient, which is the calibration parameter. The dispersion factor accounts for the process of mixing salinity between two neighboring parcels of water.

DSM2-QUAL's current set of dispersion factors used in simulating the transport of salinity in the Delta were calibrated to measured EC. In the calibration process, dispersion factors are typically adjusted until the annual peak salinity at upstream locations is reproduced in the late summer or fall. Thus, the calibration is naturally focused on periods when boundary EC will be highest. This adjustment to the dispersion factor can result in erroneous outputs in wetter conditions when EC in Suisun Bay is much lower (Suits, 2002).

EC was selected as the parameter for calibration as EC data is available in abundance in the Delta. EC is recorded every 15 minutes or hourly at multiple sites within the Delta and data extend back to the 1980s or earlier, depending upon the site. Other potential constituents for calibration, such as chloride and total dissolved solids (TDS), are far less available in the Delta and would have to be inferred from relationships to EC (Suits, 2002).

2.3 DSM2 Historical Simulation Model

California Department of Water Resources (DWR) maintains a DSM2 simulation of recent historical conditions as an ongoing check of the ability of the model to reproduce the actual measured flows and salinity in the Delta. DWR uses the recent historical simulation to support water quality forecasting for compliance. In this study, the inputs for the most recent historical hydrodynamic and water quality simulations are used. This study evaluated only the water quality simulation module, DSM2-QUAL where the required input files provided by DWR Bay Delta Office (BDO) were used for generating the hydrodynamic data for running the DSM2-QUAL module.

3.0 Methodology

This chapter describes the methodology and data used to complete this validation evaluation effort.

3.1 Anions and Cations Evaluated

The following seven different cations and anions were used in this study to evaluate the ability of the DSM2 model to simulate other salinity constituents:

- Calcium
- Magnesium
- Sodium
- Alkalinity (bicarbonate)
- Chloride
- Bromide
- Sulfate

Input data for these cations and anions were made available by DWR BDO.

EC was used in this study to enable a comparison of EC results with the results for other cations and anions.

3.2 Delta Locations

A list of locations in the Delta selected for validating the model is presented in Table 1. Figure 1 shows the six locations in the Delta selected for validating the model. After a detailed review of the existing data sets from Interagency Ecological Program (IEP) and DWR water data library, the following data sets were identified for the selected locations in the Delta. Table 1 presents a summary of the observed cation and anion data at the selected Delta locations.

Table 1. Summary of Available Validation Data in the Six Delta Locations

Location	Station Description[1]	Station ID[1]	Beginning Date	Ending Date	DSM2 Channel Name	DSM2 Channel
Jones Pumping Plant	DMC Intake at Lindemann Rd.	B9C74901336	26-Jul-83	26-May-99	chdmc004	216
Banks Pumping Plant	Clifton Court Intake	KA000000	26-Jul-83	18-Apr-11	chswp003	82
Old River at Bacon Island	Old River at Bacon Island	B9D75811344	17-Nov-94	2-May-11	rold024	106
San Joaquin River at Jersey Point	San Joaquin River at Jersey Point	B9D80311413	10-Jul-90	14-Jun-95	rsan018	83
Sacramento River at Mallard Island	Sacramento River at Mallard Island	E0B80261551	8-May-85	2-May-11	rsac075	437
San Joaquin River at Highway 4	San Joaquin River at Hwy. 4	B9D75571196	19-Jul-88	7-Aug-01	rsan063	90

Source: [1] DWR Water Data Library

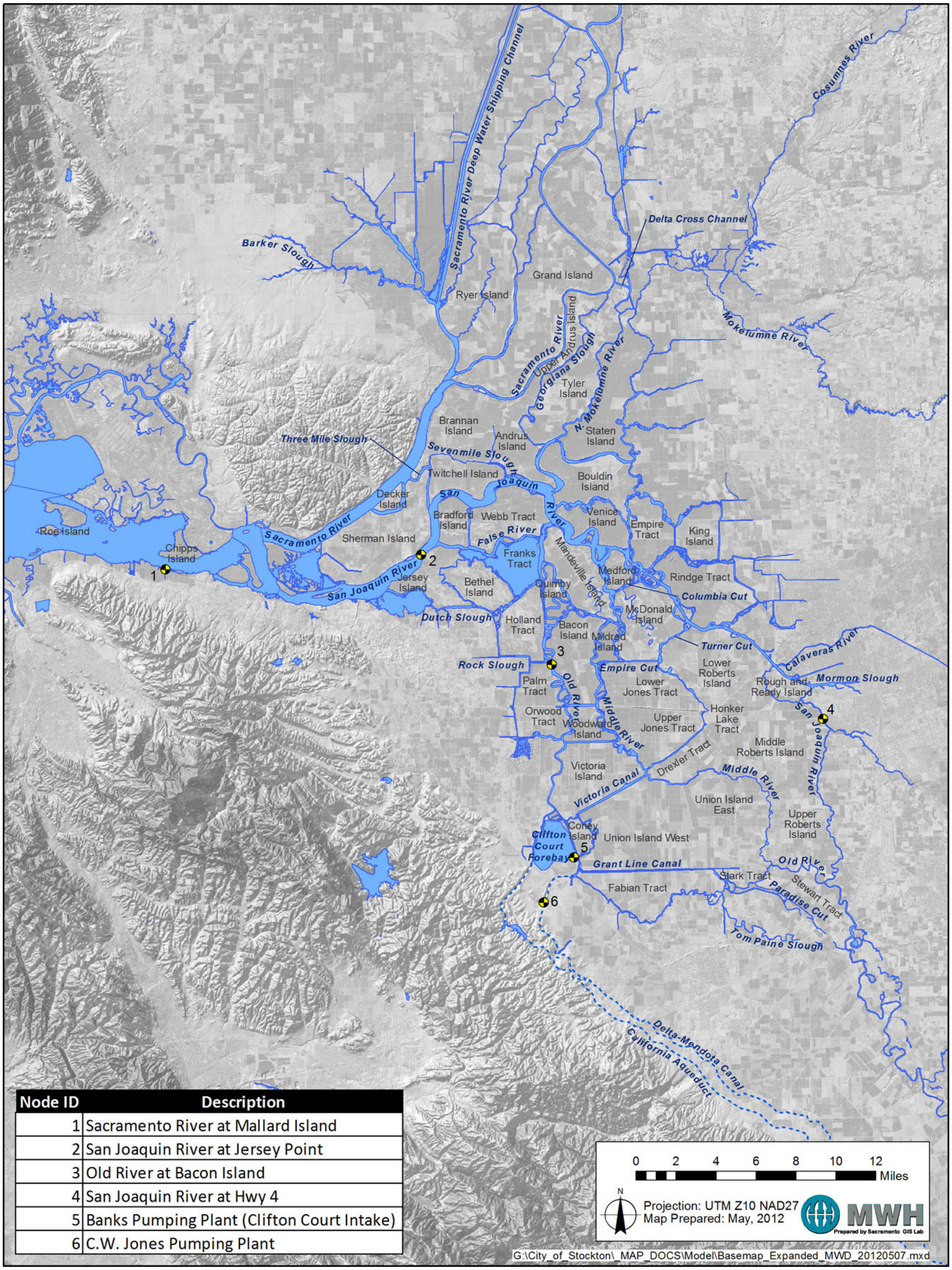

Figure 1. Map showing Locations in the Delta for Validating the Model

3.3 Boundary Water Quality

EC boundary conditions were developed by BDO from grab sample data on a daily time step. Boundary conditions for the seven water quality parameters modeled were generated using regression equations developed by BDO. Tables 2 and 3 present the regression coefficients used in Equation 1 for calculating the daily concentrations for each of the seven water quality parameter from daily EC values.

$$Anion\ or\ Cation\ concentration\ in \frac{mg}{l} = A + B * EC + C * EC^2 \qquad (1)$$

Where EC is electrical conductivity in micro Siemens per centimeter (µS/cm)

Boundary conditions of Delta island return flow quality are based upon a memorandum report (DWR, 1995) for the water quality parameters.

Table 2. Regression Coefficients/Constants for Sacramento and San Joaquin River Boundary Conditions

Constituent	Sacramento River Boundary (Includes Yolo Bypass)			San Joaquin River Boundary		
	A	B	C	A	B	C
Calcium	3.76	0.0513	0	2.18	0.0466	0
Magnesium	0.141	0.0403	0	0.305	0.0244	0
Sodium	-4.23	0.0904	0	-5.78	0.12	0
Alkalinity	6.46	0.33	0	6.8	0.173	-0.0000437
Bromide	-0.022	0.000297	0	-0.046	0.000471	0
Chloride	-3.8	0.0698	0	-6.16	0.12	0.000047
Sulfate	-1.4	0.0656	0	4.6	0.0907	0.0000459

Table 3. Regression Coefficients/Constants for East Side Streams and Tidal Boundary Conditions

Constituent	East Side Stream Boundaries			Tidal Boundary (ignore low salinity condition)		
	A	B	C	A	B	C
Calcium	-1.4	0.113	0	11.52	0.0068	0
Magnesium	-1.06	0.052	0	-1.55	0.0229	0
Sodium	0.875	0.0214	0.000265	-45.86	0.179	0
Alkalinity	-1.85	0.396	0	64.97	0.00125	0
Bromide	-0.022	0.000297	0	-0.442	0.00118	0
Chloride	0.105	0.0545	0	0	0.299	0.0000018
Sulfate	-2.18	0.101	0	-5.75	0.0446	0

3.4 Boundary Water Quality Data Verification

The quality of the water quality data generated using the regression equations was verified using cation-anion charge balance analysis. It is based on the theory that the total cation and anion charges in the different sources of Delta water, when expressed as milli-equivalents per liter (meq/L), must balance to maintain electrical neutrality.

Tables 4 and 5 show the results of cation-anion balance calculations for Sacramento and San Joaquin River water, respectively. Cation and anion charges presented in Table 4 do not account for minor constituents that may explain minor differences. As reported by Hem (1985), total cation or anion (100 x meq/L) approximately equals EC in µs/cm which is described as EC-to-charge ratio, which is also used in verifying the consistency of water quality data.

Table 4. Cation-Anion Balance for Sacramento River Water

Observed Electrical Conductivity (µS/cm)	Charge (meq/l)			EC/Charge Ratio	
	Observed Cations[1]	Observed Anion[2]	Difference (%)	Cations	Anions
100	1.02	0.99	-4%	98	101
125	1.27	1.23	-3%	98	101
150	1.52	1.48	-2%	99	101
175	1.77	1.73	-2%	99	101
200	2.01	1.98	-2%	99	101
225	2.26	2.23	-1%	99	101
250	2.51	2.48	-1%	100	101
275	2.76	2.73	-1%	100	101
300	3.00	2.97	-1%	100	101

Notes:
[1] Sodium, Calcium and Magnesium
[2] Chloride, Bromide, Sulfate and Alkalinity (Bicarbonate)
Key:
EC = electrical conductivity
meq/l = milliequivalent per liter
µS/cm = micro Siemens per centimeter

Table 5. Cation-Anion Balance for San Joaquin River Water

Observed Electrical Conductivity (µS/cm)	Charge (meq/l)			EC/Charge Ratio	
	Observed Cations[1]	Observed Anion[2]	Difference (%)	Cations	Anions
100	0.86	0.95	9%	116	106
200	1.83	1.86	2%	109	107
300	2.79	2.81	0%	107	107
400	3.76	3.78	1%	106	106
500	4.72	4.78	1%	106	105
600	5.69	5.81	2%	106	103
700	6.65	6.86	3%	105	102
800	7.62	7.95	4%	105	101
900	8.58	9.06	6%	105	99
1000	9.54	10.20	7%	105	98
1100	10.51	11.37	8%	105	97
1200	11.47	12.57	10%	105	95
1300	12.44	13.80	11%	105	94
1400	13.40	15.05	12%	104	93
1500	14.37	16.33	14%	104	92
1600	15.33	17.64	15%	104	91
1700	16.30	18.98	16%	104	90

Notes:
[1] Sodium, Calcium and Magnesium
[2] Chloride, Bromide, Sulfate and Alkalinity (Bicarbonate)
Key:
meq/l = milliequivalent per liter
µS/cm = micro Siemens per centimeter

A charge balance analyses on the total calculated cations and anions for the Sacramento River water using the regression equations showed that the results are reasonably accurate at various levels of salinity. The total calculated anion charges are higher than the total calculated cations charges in the San Joaquin River, especially when the salinity levels in the San Joaquin River exceeds 1000 µS/cm. However, salinity in the San Joaquin River has exceeded the current regulatory standard of 1,000 µS/cm only during 4 percent of the time between January, 1990 and December, 2010, based on the EC San Joaquin River boundary data used in the model. Similarly, cation-anion charge balance analyses of west Delta water indicated that the total anion charges are greater than the total cation charges by up to 18 percent at high salinity concentrations.

Figures 2 and 3 compares typical ocean salinity and computed ocean salinity at high values of TDS, based on ionic concentrations. From Figures 2 and 3, it can be seen that the computed ionic concentrations are comparable to typical values. Overall, the regression equations available for translating EC values to the other water quality parameter values for the different sources of Delta water are shown to be valid and justifiable for generating the necessary boundary conditions for DSM2.

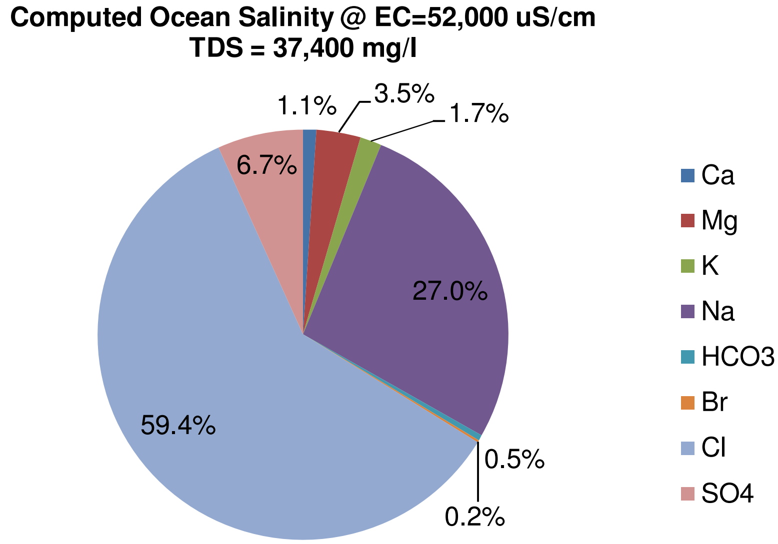

Figure 2. Computed Ocean Salinity

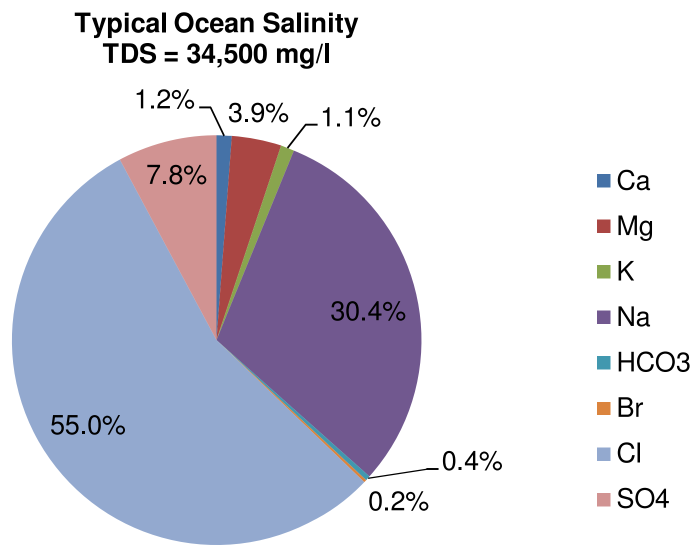

Figure 3. Typical Ocean Salinity

Daily observed water quality data for San Joaquin River at Vernalis were downloaded from California Data Exchange Center (CDEC). Figures 4 through 7 show a comparison of observed data and the DSM2 boundary data for EC, chloride, bromide and sulfate concentrations in San Joaquin River at Vernalis. It is noted that 4 out of 880 grab samples (< 1%) recorded bromide concentrations greater than 1 mg/L. These observations which are probably data outliers are not represented in the DSM2 boundary conditions. Overall, it is shown that the boundary conditions of San Joaquin River water quality at Vernalis are represented adequately in the DSM2 historical simulation.

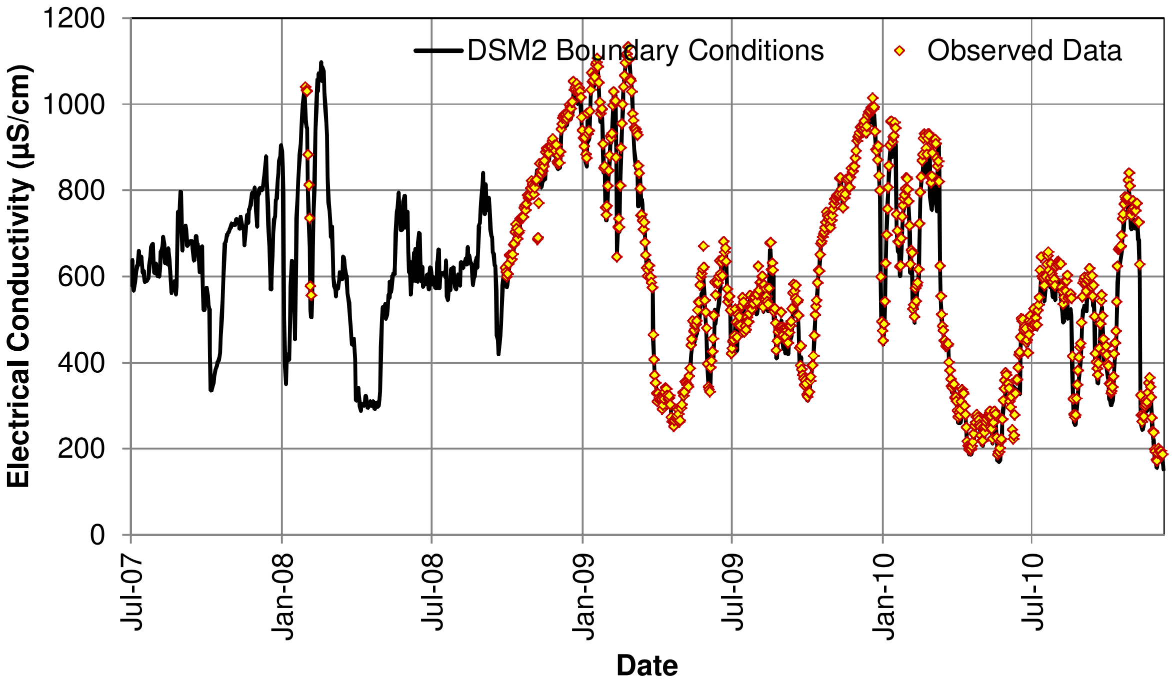

Figure 4. Comparison of DSM2 Boundary and Observed Daily Data for Electrical Conductivity in the San Joaquin River at Vernalis

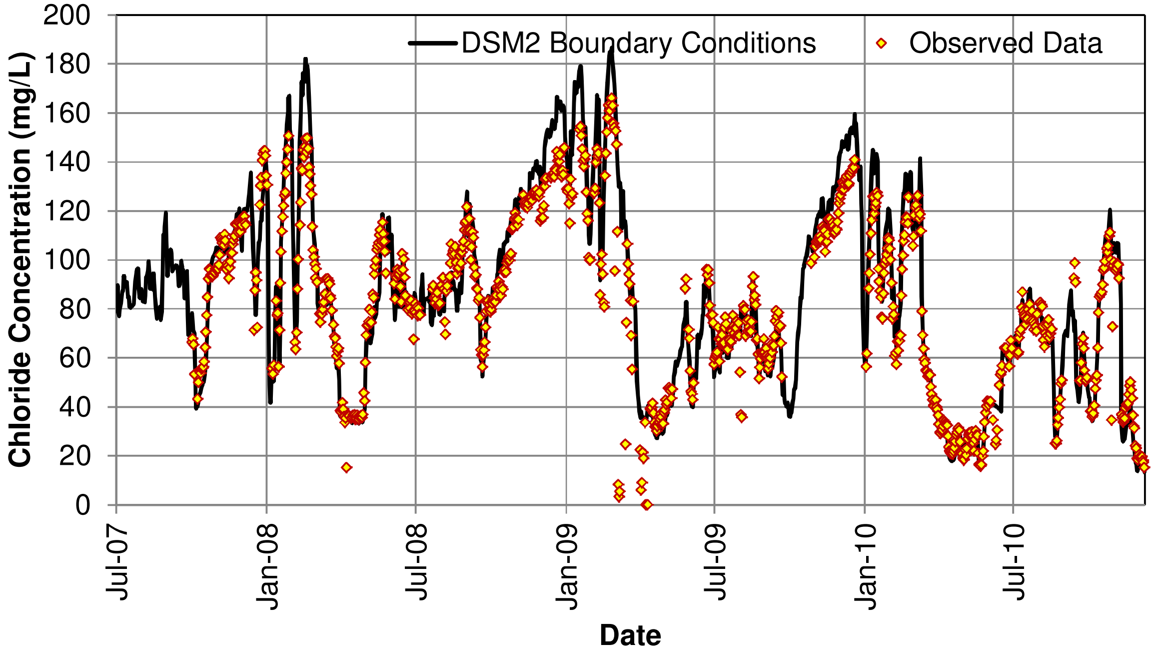

Figure 5. Comparison of DSM2 Boundary and Observed Daily Data for Chloride Concentrations in the San Joaquin River at Vernalis

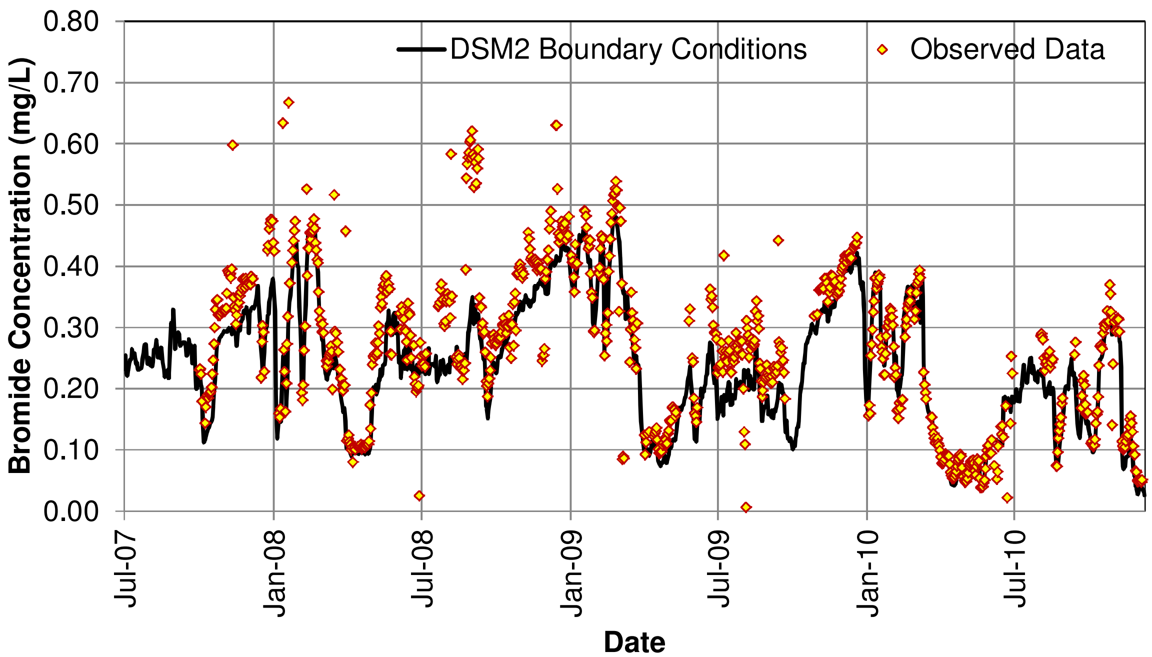

Figure 6. Comparison of DSM2 Boundary and Observed Daily Data for Bromide Concentrations in the San Joaquin River at Vernalis

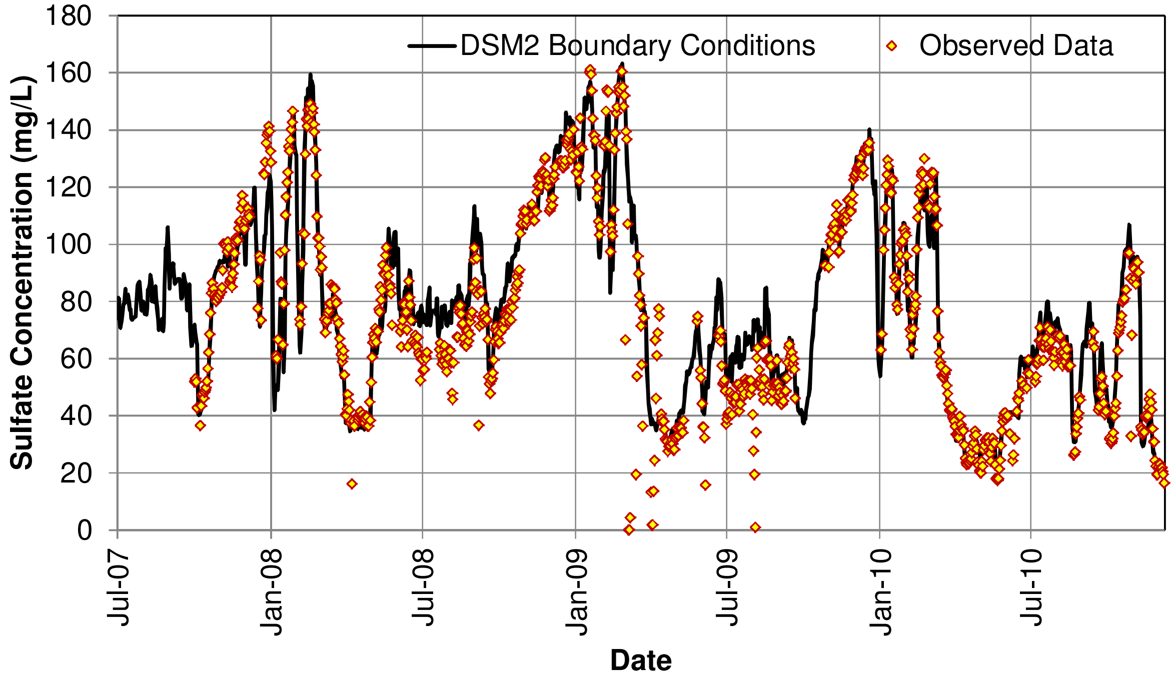

Figure 7. Comparison of DSM2 Boundary and Observed Daily Data in San Joaquin River for Sulfate Concentrations at Vernalis

3.5 Model Validation

The following section discusses the methods followed in this study to validate the DSM2 model (Version 8.0.4) for simulation of various cations and anions. The historical simulation covered the period from January 1, 1990, through December 31, 2010, which includes a 5-month "warm-up" period that allows for adequate mixing of the initial boundary conditions within DSM2. Historical simulation results for cations, anions, and EC were output in 15-minute, daily, and monthly formats for selected output locations.

Although model outputs are available at different time steps, the lack of adequate grab sample data for the water quality parameters (except EC) rendered a traditional daily or monthly analysis challenging. Therefore, model validation was performed by comparing available grab sample data against model outputs available at the nearest time interval to the sample collection date and time. All further analyses described in this report are based on comparing grab sample data and 15-minute water quality outputs from DSM2, unless noted otherwise.

In this validation exercise, three different error functions (the root mean square error (RMSE), normalized root mean square error (NRMSE) and bias (mean error) are used to evaluate the model performance described in Equations 2, 3, and 4.

The RMSE of a model prediction with respect to the estimated variable X_{model} is defined as the square root of the mean squared error:

$$RMSE = \sqrt{\sum_1^n \frac{(X_{obs} - X_{model})^2}{n}} \qquad (2)$$

where X_{obs} is the observed value and X_{model} is the modeled value available at the date and time of collection of the grab sample data and n refers to the number of samples.

NRMSE is the RMSE divided by the range of observed values, which are dimensionless and are used to compare between the model results of different cations and anions.

$$NRMSE = \frac{RMSE}{({X_{obs}}^{max} - {X_{obs}}^{min})} \qquad (3)$$

Bias is the average error between observed and modeled results and is used to assess if the model is overestimating or underestimating the observed values.

$$Bias = \sum_1^n \frac{(X_{obs} - X_{model})}{n} \qquad (4)$$

Model performances were also assessed using scatter plots and time-series plots at each of the six Delta locations mentioned earlier. Scatter plots are used for the validation purposes to see how well the model results correspond to the observed data in terms of direction (overestimating or underestimating) of plotted data and data trends, etc. Scatter plots are also useful in identifying data outliers.

4.0 Results and Discussions

This chapter describes the model validation results for EC and other cations and anions.

4.1 Electrical Conductivity

Historical efforts on EC validation have led to the conclusions that EC results agreed well with the observed data at most of the locations in the Delta. Thein and Nader-Tehrani, (2006) reported that annual peak EC values in the Delta that generally occurred during the fall or early winter periods were captured fairly well by DSM2. As a general trend, DSM2 was found to overestimate EC in most summers of dry periods (Thein and Nader-Tehrani, 2006). Although, the DSM2 model has been validated by earlier studies, this study validated the DSM2 model based on the grab samples used for validating cations and anions.

The primary focus of this study was to validate the DSM2 model for simulation of cations and anions and not EC. Therefore, available continuous EC data in the Delta were not used in this study. By using grab sample data for EC to validate the DSM2 model, it was possible to compare the model performances in simulating EC against cations and anions based on a consistent observed data set. This comparison based on grab sample data was useful in understanding the error patterns in cation and anion simulation results and in assessing the performances of the model in simulating cations and anions relative to EC.

This section summarizes model performances in simulating EC at six Delta locations. Various summary statistics along with time-series plots and scatter plots are used to validate the DSM2 model for simulating EC in the Delta. Table 6 presents a summary of bias, RMSE and NRMSE values for EC simulations at the six locations in the Delta.

Table 6. Validation Summary Statistics for EC Simulation at Different Locations in the Delta

Locations	Average Electrical Conductivity		Bias	RMSE	NRMSE	Samples
	Observed (µS/cm)	Simulated (µS/cm)	(µS/cm)	(µS/cm)	%	
Jones Pumping Plant	537	520	17	178	18%	140
Banks Pumping Plant	463	436	27	117	13%	162
Old River at Bacon Island	376	329	47	89	10%	280
San Joaquin River at Jersey Point	1288	1626	-338	726	28%	51
Sacramento River at Mallard Island	5868	6225	-357	1515	8%	272
San Joaquin River at Highway 4	508	488	20	91	12%	47

Key:
NRMSE = normalized root mean square error
RMSE = root mean square error
µS/cm = micro Siemens per centimeter

Results in Table 6 show that DSM2 results correspond well to observed data at the six locations considered in this study, except for the San Joaquin River at Jersey Point. Table 6 shows relatively higher NRMSE values for the San Joaquin River at Jersey Point when compared to other locations. Historically, DSM2 has been shown to perform well in the San Joaquin River at Jersey Point. Reported observation of large NRMSE values does not necessarily mean that the model performed poorly at this location. Further validation with a different set of observed data can help explain these anomalous results at this location.

Figure 8 shows scatter plots for six Delta locations comparing observed EC data (y-axis) and simulated data (x-axis). It can be seen from Figure 3 that there are some inconsistencies in the simulation of EC at varying levels of salinity conditions. As shown in Figure 8, data points at higher salinity concentrations are more scattered around the best fitting line, which indicates that large residual errors may be associated with the period of higher relative salinity at each location. Results in Table 6 as well as the scatter plots also show that the model underestimates EC at south Delta locations and overestimates in the Sacramento River at Mallard Island.

Figures 9 through 14 show the time-series plots of grab sample data and simulated daily average EC at the six Delta locations. Figures 9 through 14 also show that the model captures the seasonal and temporal trend of the observed data well at the six Delta locations.

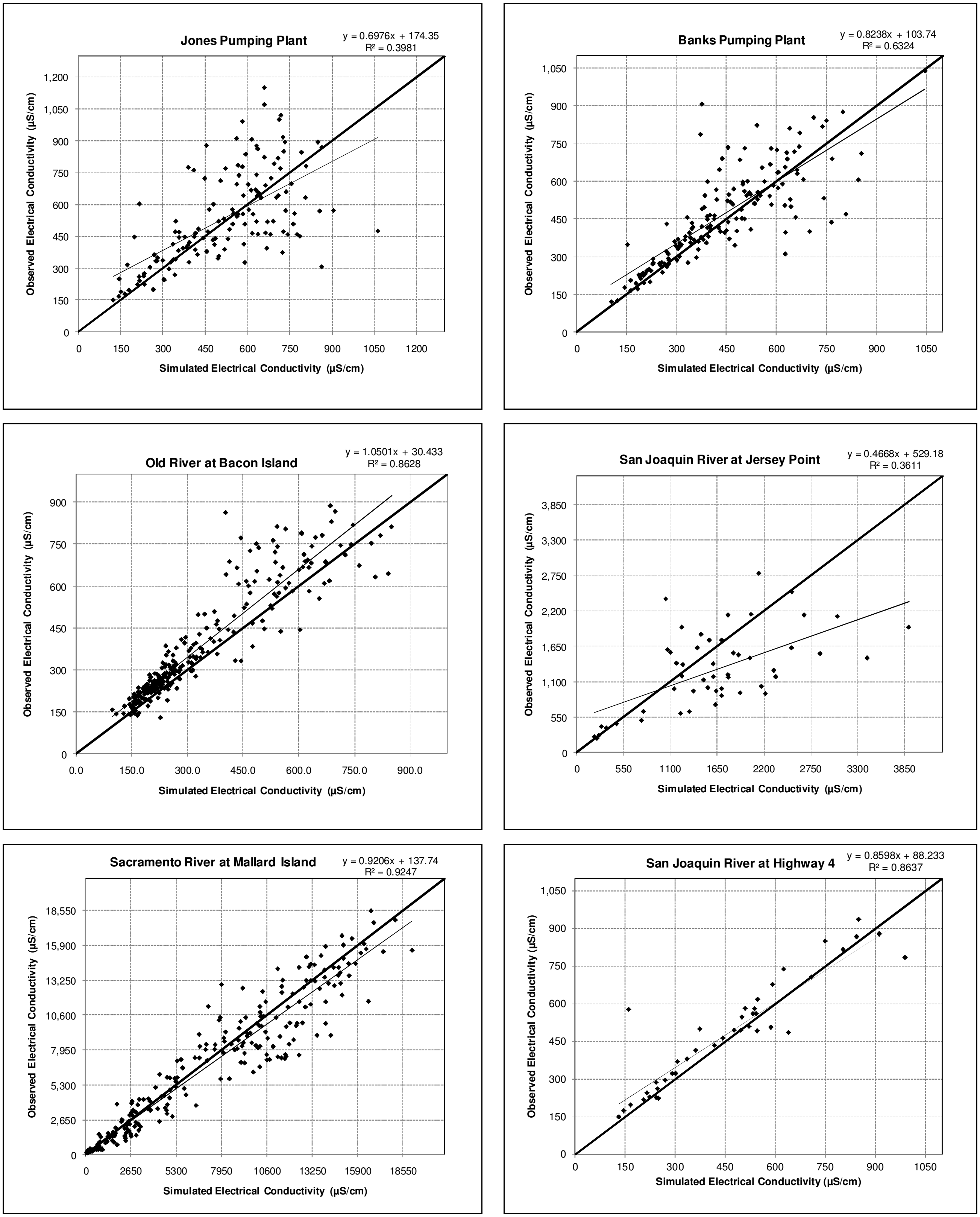

Figure 8. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

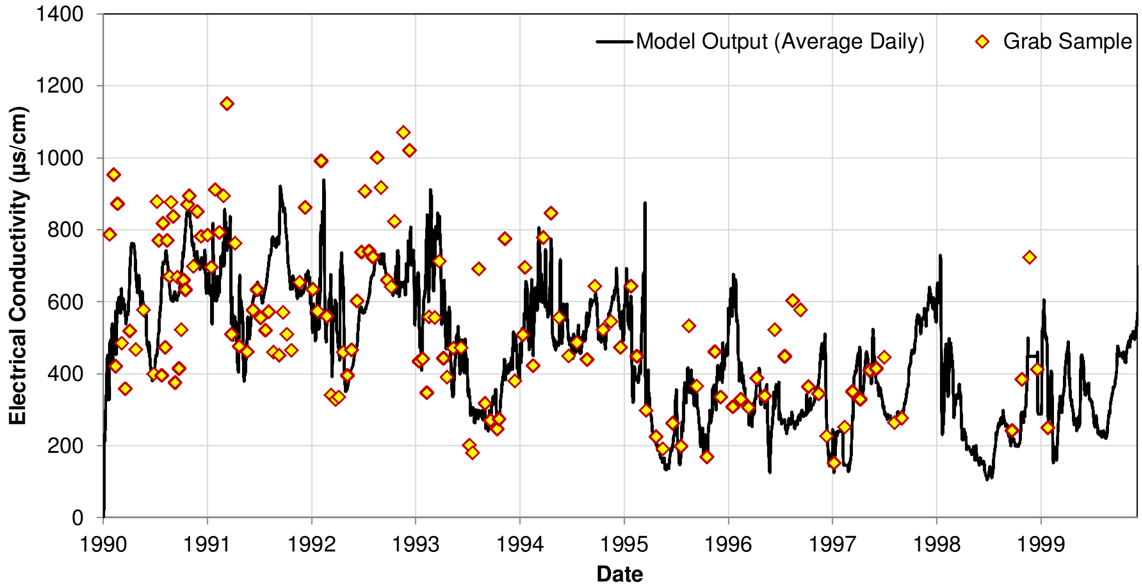

Figure 9. Comparison of Grab Sample Data and Simulated Daily Average EC Values at Jones Pumping Plant

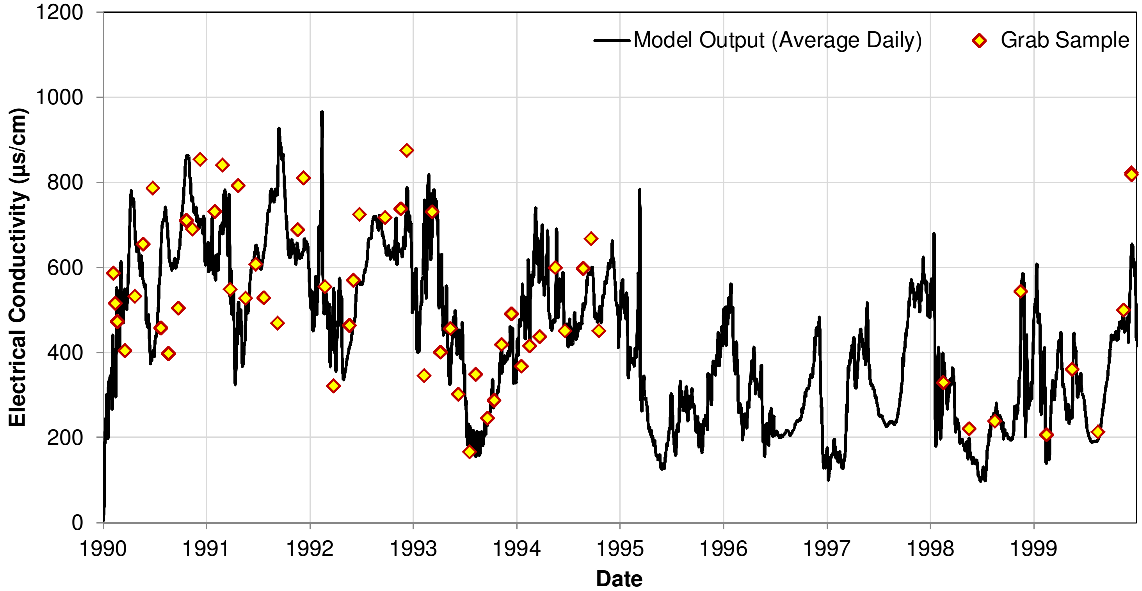

Figure 10a. Comparison of Grab Sample Data and Simulated Daily Average EC Values at Banks Pumping Plant

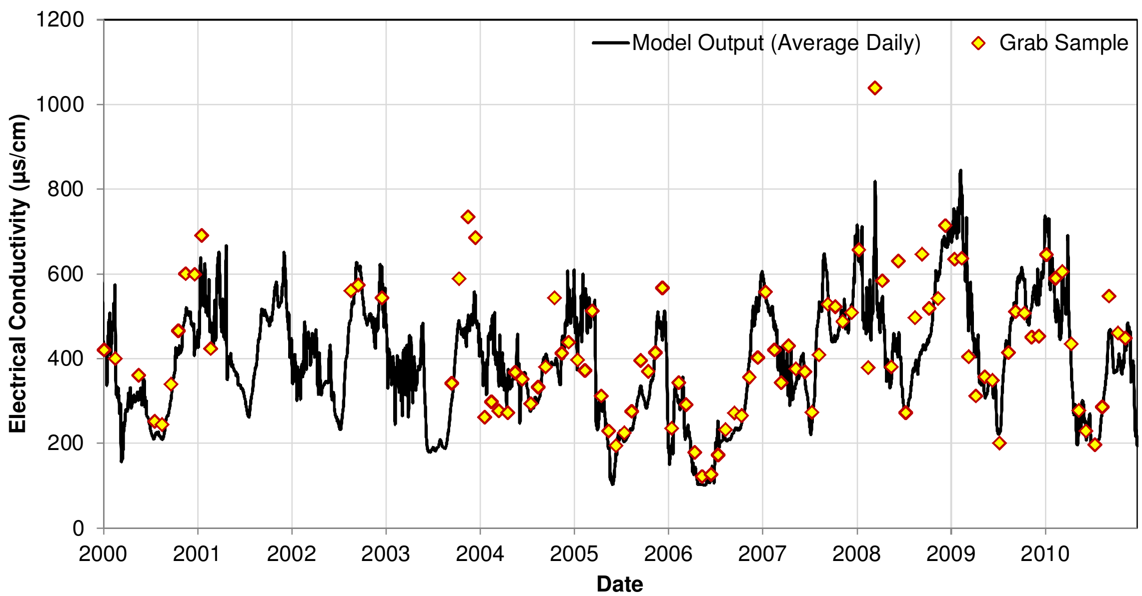

Figure 10b. Comparison of Grab Sample Data and Simulated Daily Average EC Values at Banks Pumping Plant

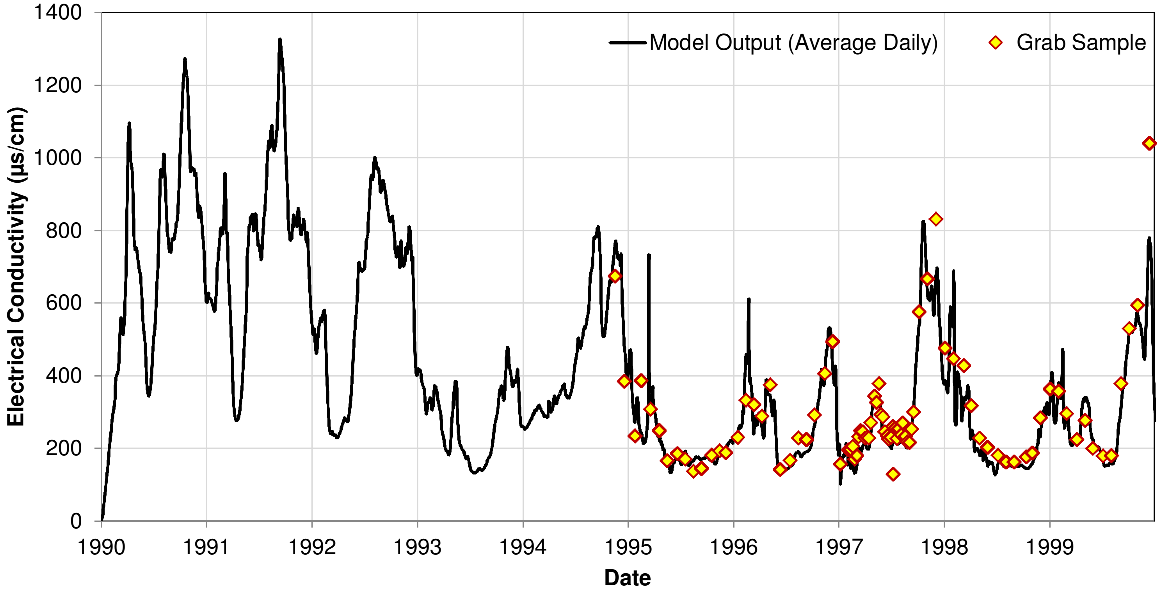

Figure 11a. Comparison of Grab Sample Data and Simulated Daily Average EC Values in Old River at Bacon Island

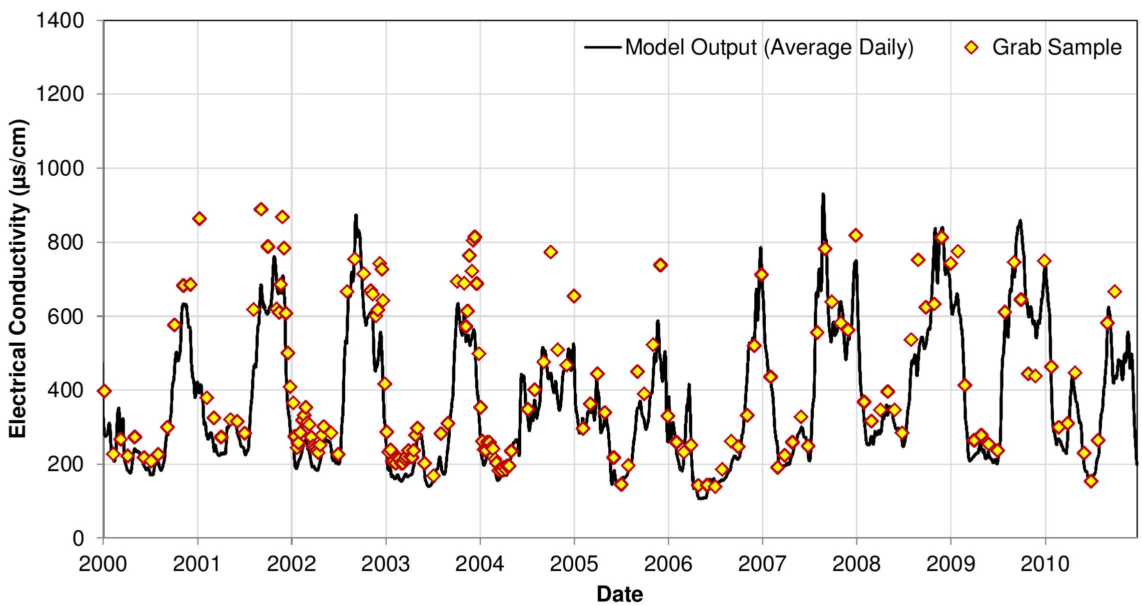

Figure 11b. Comparison of Grab Sample Data and Simulated Daily Average EC Values in Old River at Bacon Island

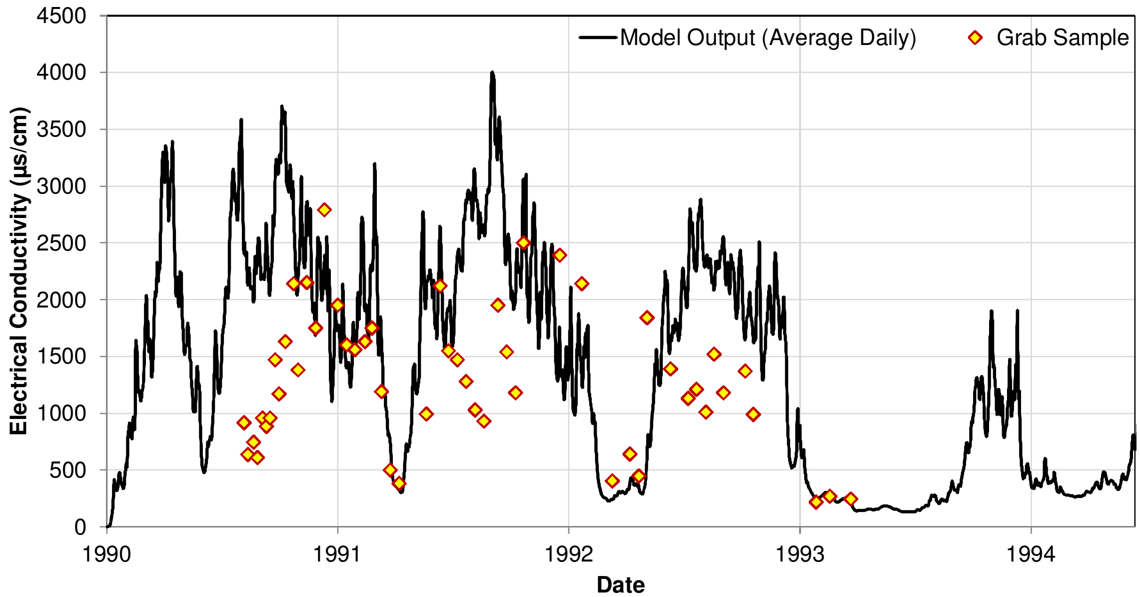

Figure 12. Comparison of Grab Sample Data and Simulated Daily Average EC Values in San Joaquin River at Jersey Point

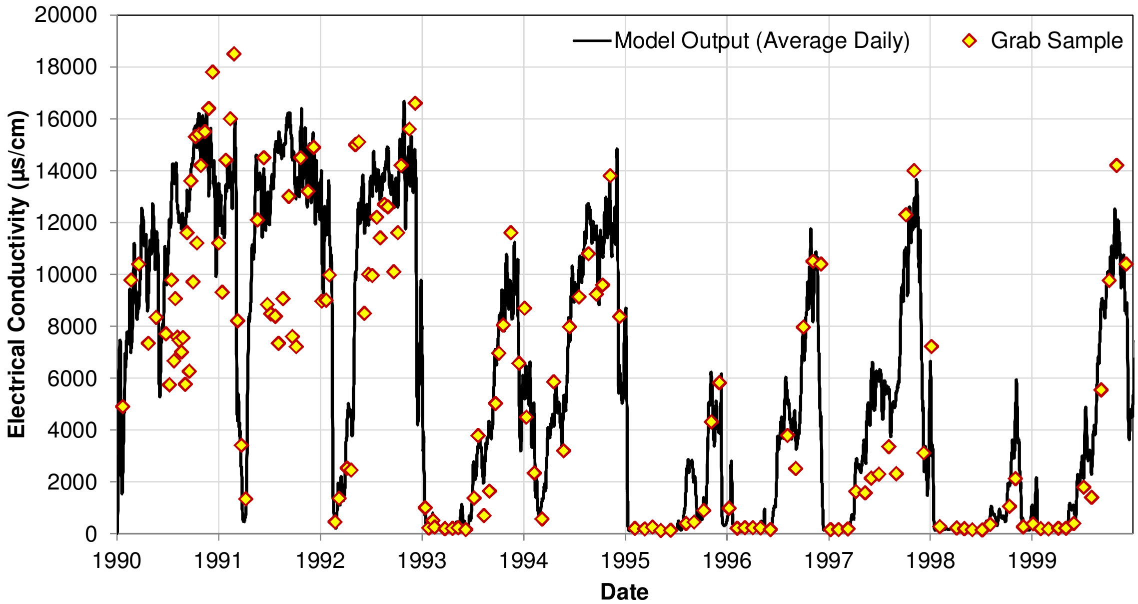

Figure 13a. Comparison of Grab Sample Data and Simulated Daily Average EC Values in Sacramento River at Mallard Island

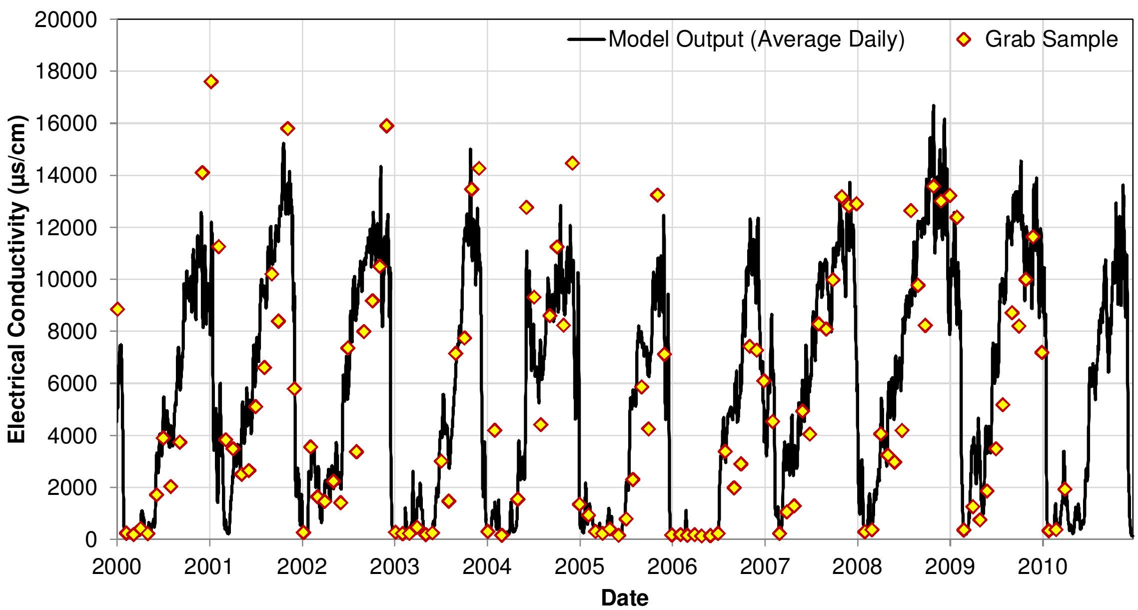

Figure 13b. Comparison of Grab Sample Data and Simulated Daily Average EC Values in Sacramento River at Mallard Island

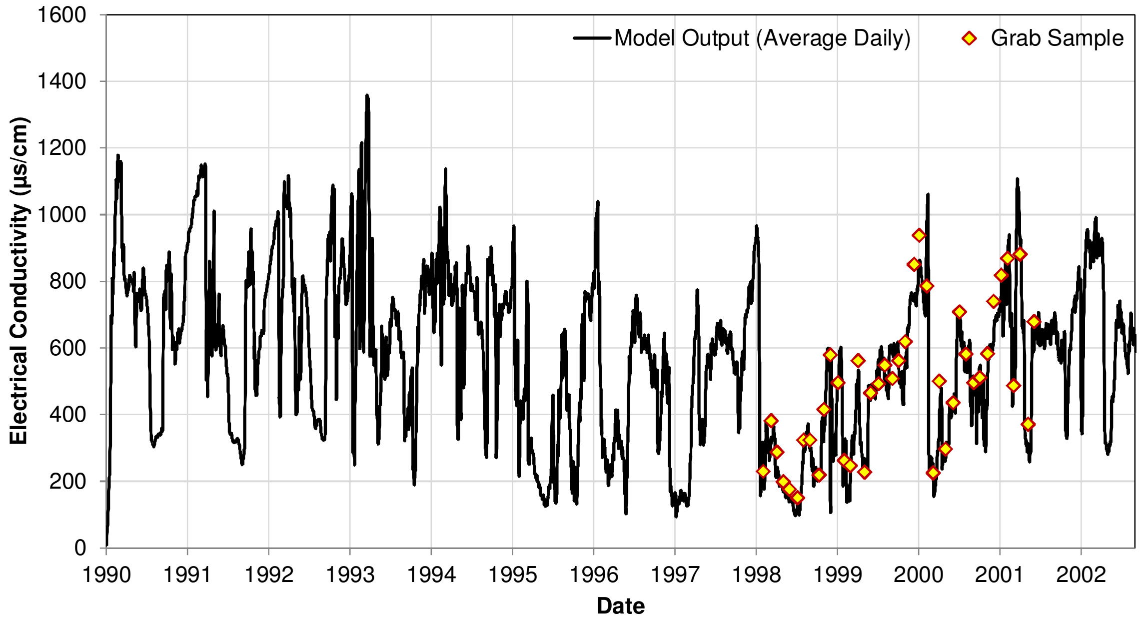

Figure 14. Comparison of Grab Sample Data and Simulated Daily Average EC Values in San Joaquin River at Highway 4

4.2 Chloride

This section provides a summary of model performances in simulating chloride concentrations at six Delta locations. Table 7 presents a summary of Bias, RMSE and NRMSE values for chloride simulations at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that the DSM2 model simulates chloride concentrations in the Delta reasonably well except in San Joaquin River at Jersey Point. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. Average Bias values in Table 7 indicate that there is a general trend of overestimation of observed chloride concentrations at the six locations in the Delta which can be also seen in the scatter plots presented in Figure 15. Figures 16 through 21 show the time-series plots of grab sample data and simulated daily average chloride concentrations at the six Delta locations. From Figures 16 through 21, it can be seen that the model outputs follow the trend in observed data well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating chloride concentration at lower salinity levels than at higher salinity levels.

Table 7. Validation Summary Statistics for Chloride Simulation at Different Locations in the Delta

Locations	Average Chloride Concentration		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	81.75	95.84	-14.08	40.08	24%	142
Banks Pumping Plant	73.54	77.68	-4.14	26.54	15%	156
Old River at Bacon Island	65.84	69.02	-3.18	24.84	10%	292
San Joaquin River at Jersey Point	314.12	457.20	-143.08	257.77	35%	51
Sacramento River at Mallard Island	1859.57	2077.92	-218.36	615.40	10%	269
San Joaquin River at Highway 4	61.95	64.59	-2.64	16.74	14%	41

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

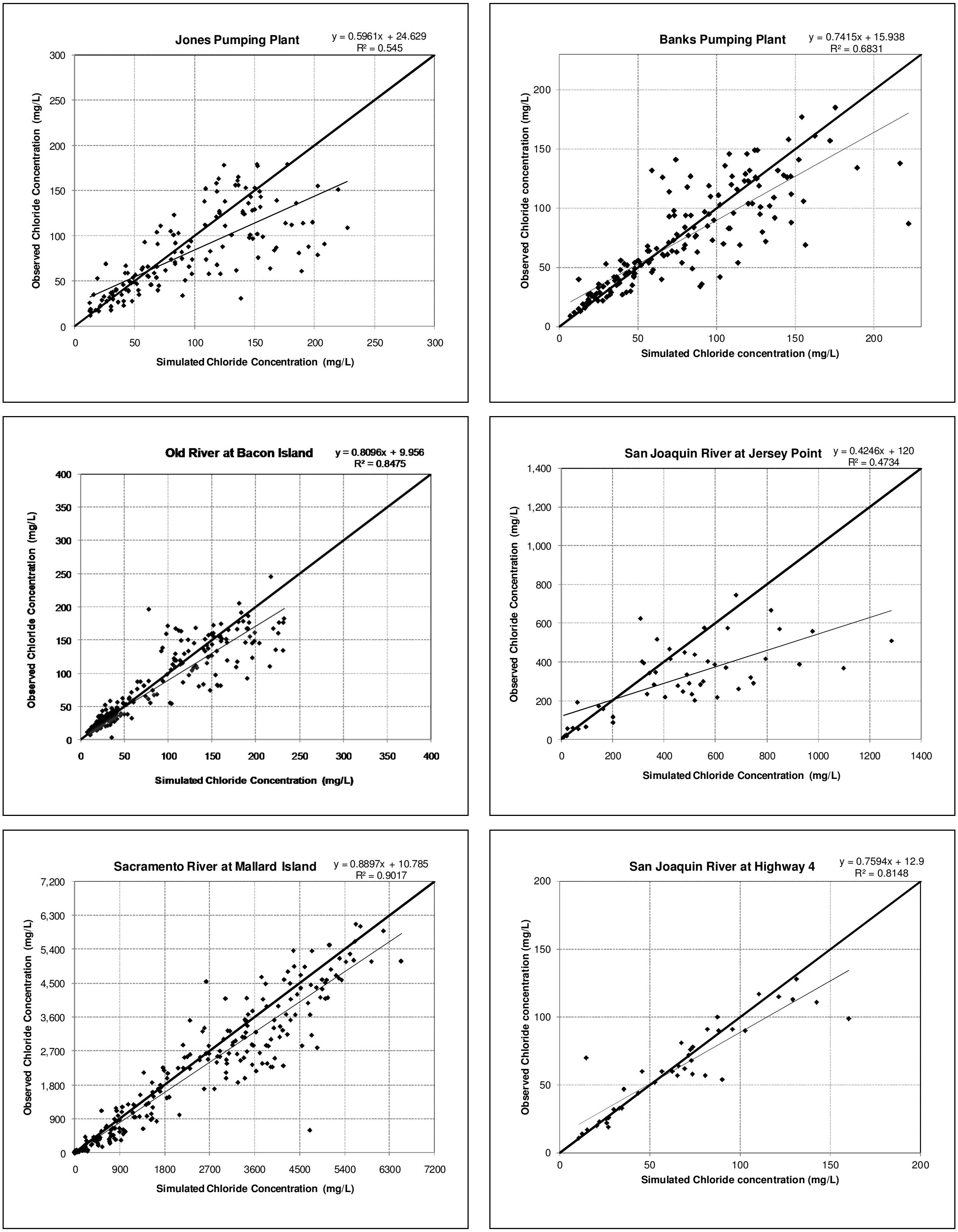

Figure 15. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

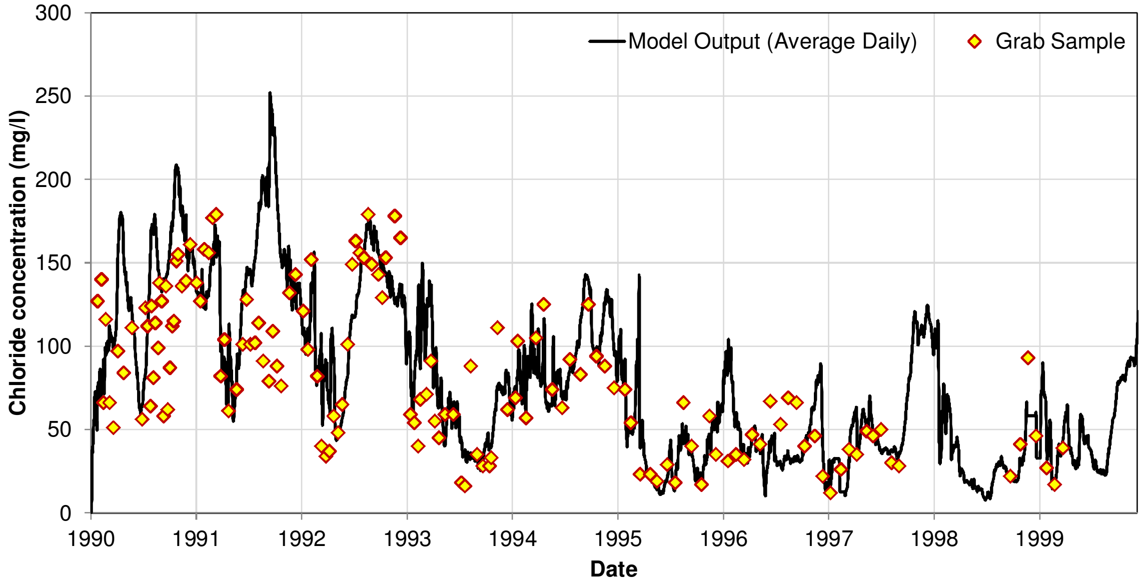

Figure 16. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration at Jones Pumping Plant

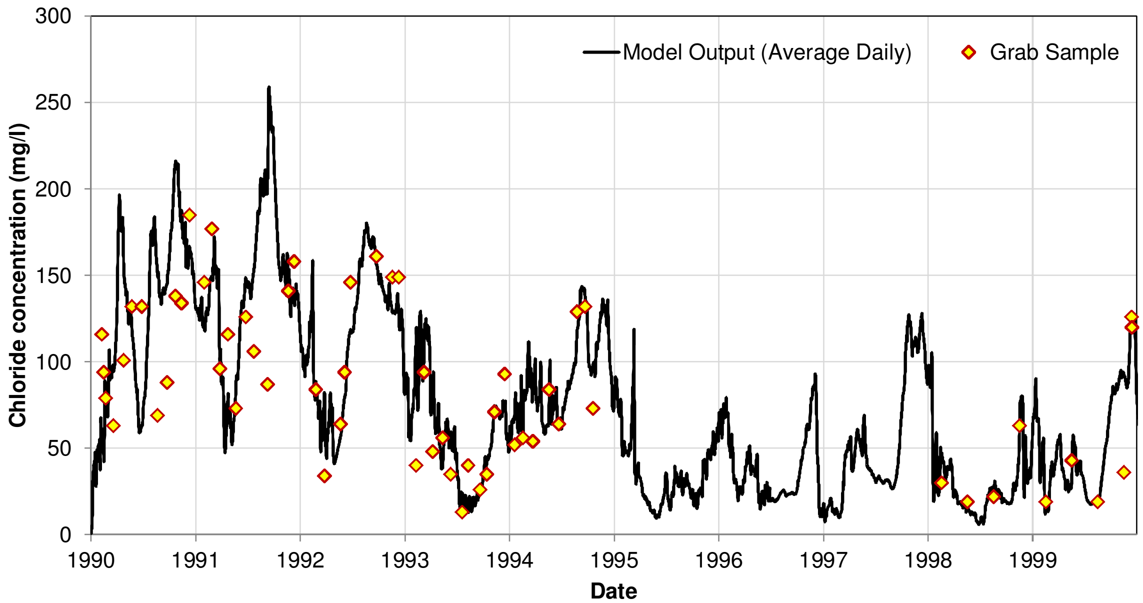

Figure 17a. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration at Banks Pumping Plant

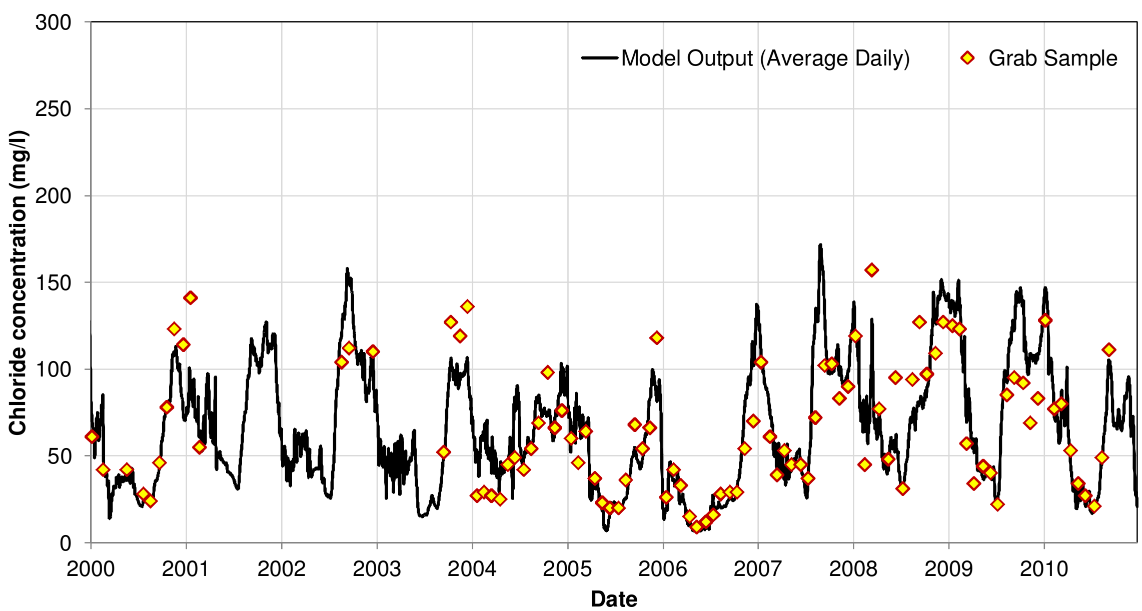

Figure 17b. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration at Banks Pumping Plant

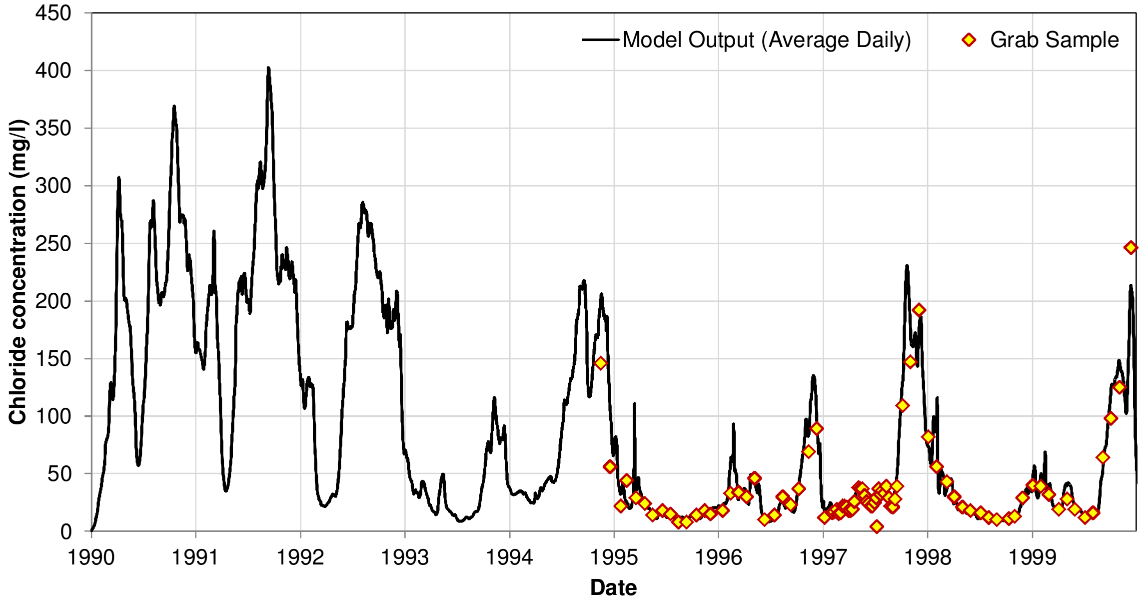

Figure 18a. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration in Old River at Bacon Island

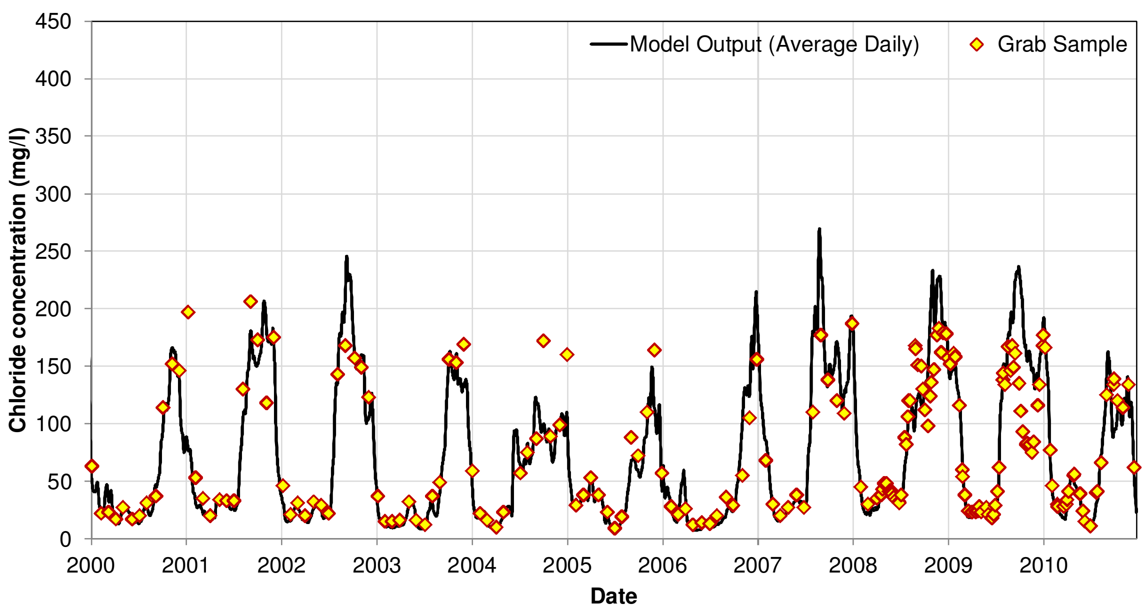

Figure 18b. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration in Old River at Bacon Island

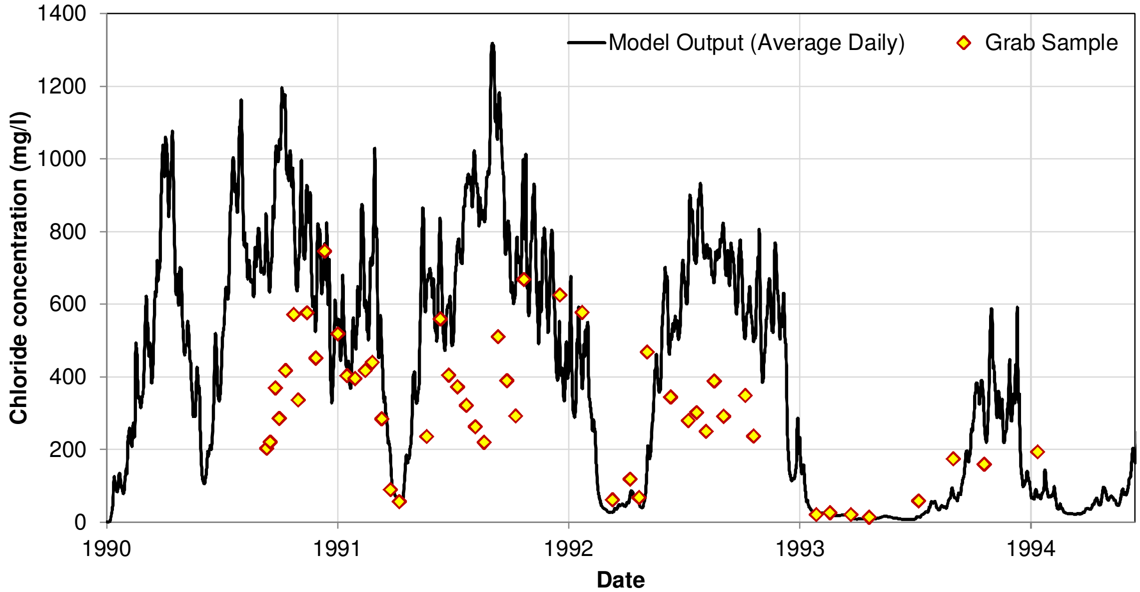

Figure 19. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration in San Joaquin River at Jersey Point

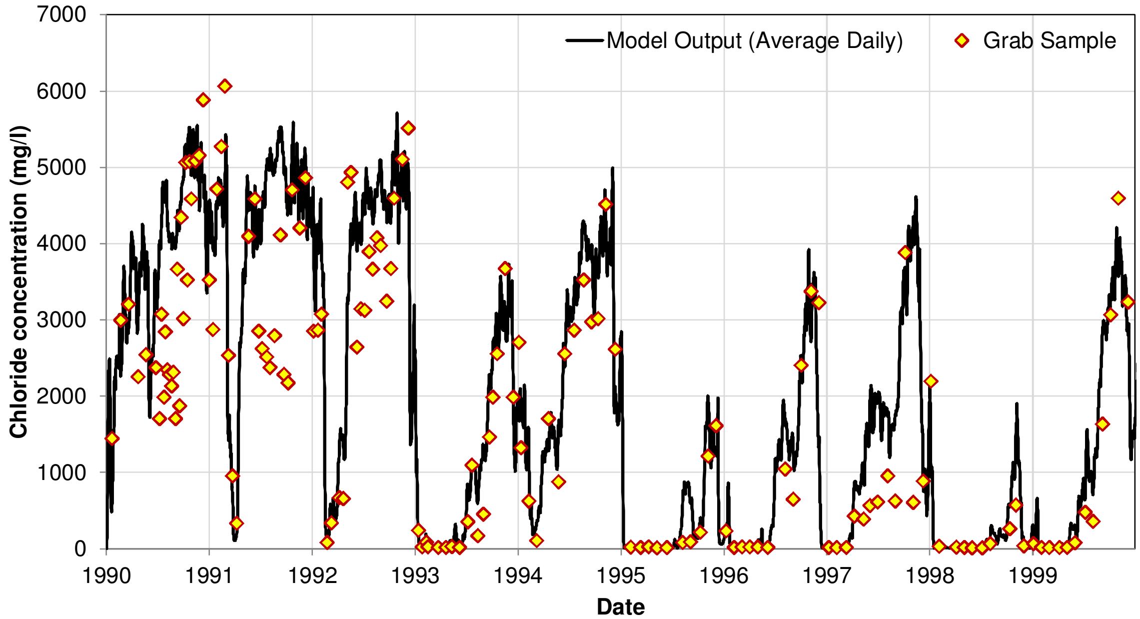

Figure 20a. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration in Sacramento River at Mallard Island

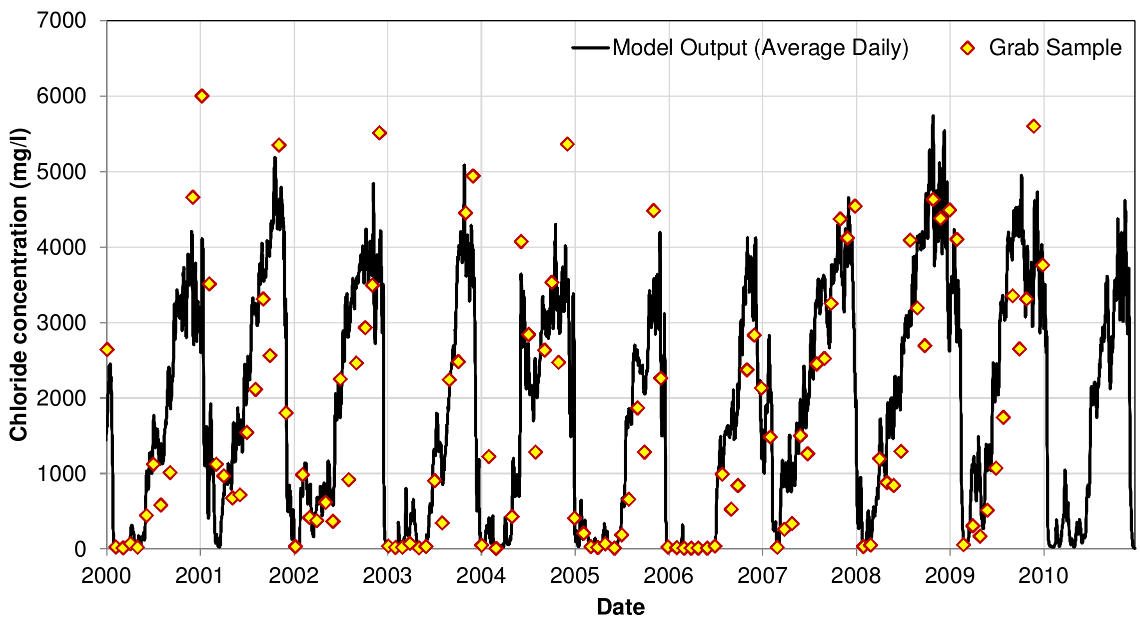

Figure 20b. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration in Sacramento River at Mallard Island

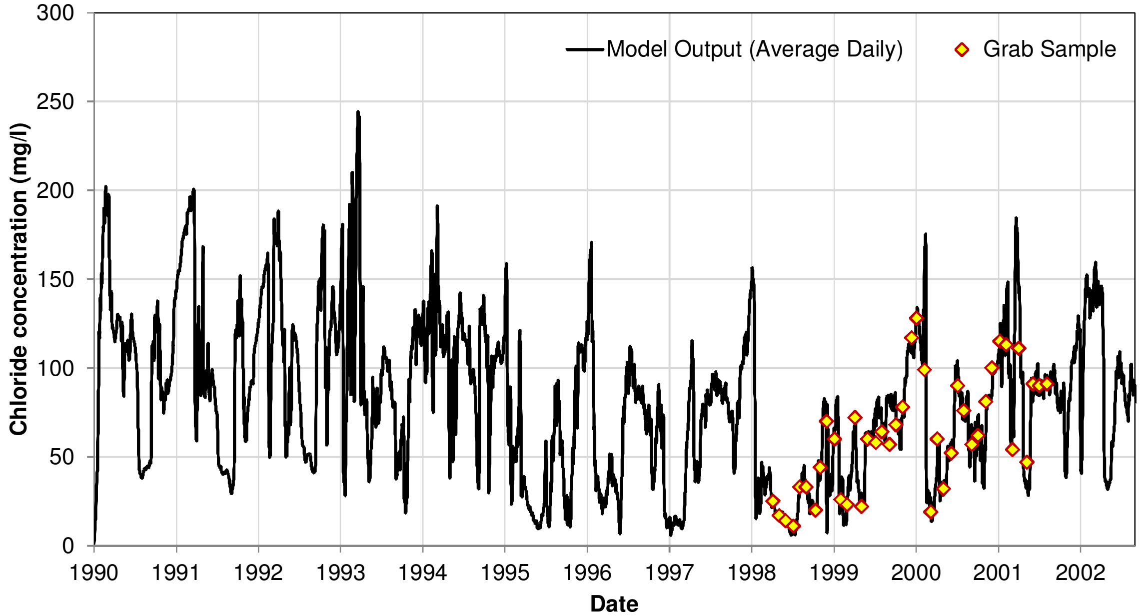

Figure 21. Comparison of Grab Sample Data and Simulated Daily Average Chloride Concentration in San Joaquin River at Highway 4

4.3 Bromide

This section provides a summary of model performances in simulating bromide concentrations at six Delta locations. Table 8 presents a summary of Bias, RMSE and NRMSE values for bromide simulations at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that the DSM2 model simulates bromide concentrations in the Delta reasonably well except in San Joaquin River at Jersey Point. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. Average Bias values in Table 8 indicate that there is a general trend of overestimation of observed bromide concentrations at the six locations in the Delta which can be also seen in the scatter plots presented in Figure 22. Figures 23 through 28 show the time-series plots of grab sample data and simulated daily average bromide concentrations at the six Delta locations. From Figures 23 through 28, it can be seen that the model outputs follow the trend in observed data well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating bromide concentration at lower salinity levels than at higher salinity levels.

Table 8. Validation Summary Statistics for Bromide Simulation at Different Locations in the Delta

Locations	Average Bromide Concentration		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	0.27	0.32	-0.05	0.13	23%	133
Banks Pumping Plant	0.22	0.25	-0.02	0.08	14%	130
Old River at Bacon Island	0.20	0.22	-0.02	0.04	5%	347
San Joaquin River at Jersey Point	1.14	1.63	-0.49	0.81	31%	53
Sacramento River at Mallard Island	6.35	6.93	-0.61	2.09	9%	273
San Joaquin River at Highway 4	0.18	0.16	0.02	0.12	34%	42

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

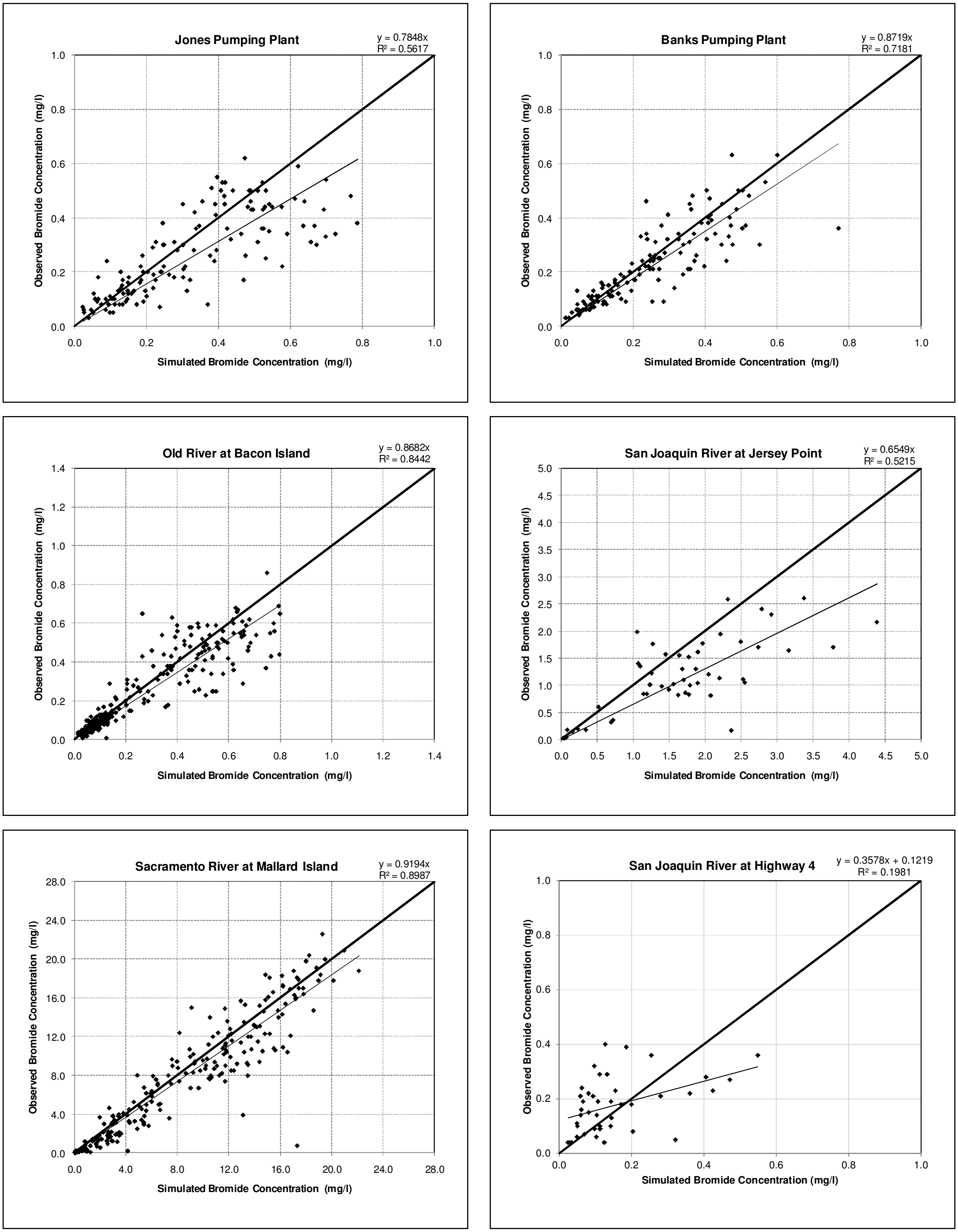

Figure 22. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

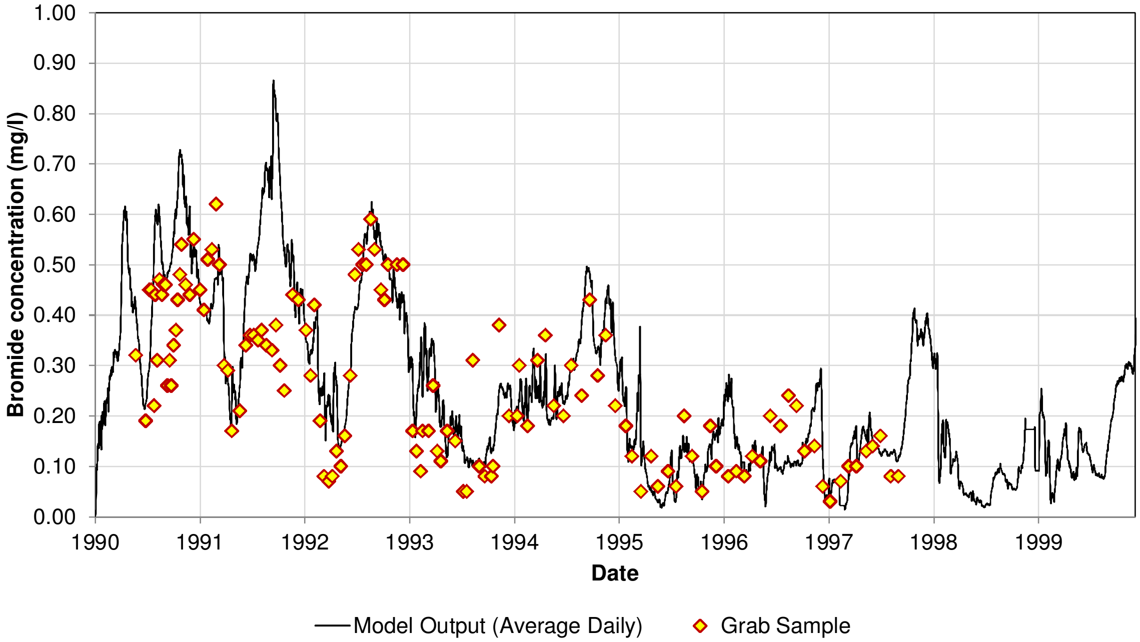

Figure 23. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration at Jones Pumping Plant

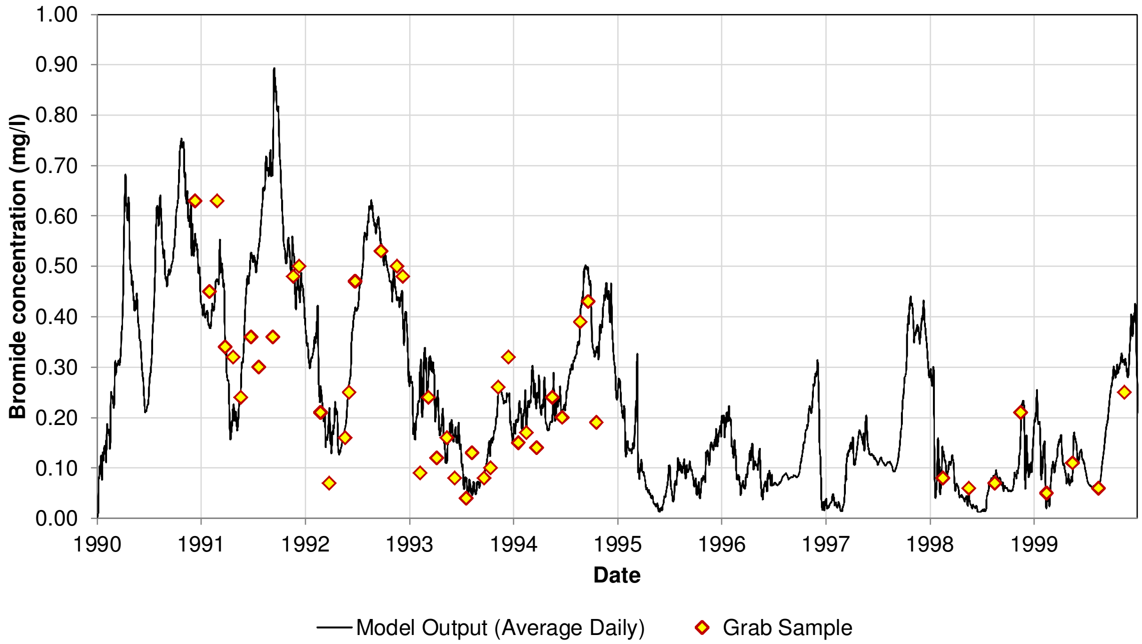

Figure 24a. Comparison Grab Sample Data and Simulated Daily Average Bromide Concentration at Banks Pumping Plant

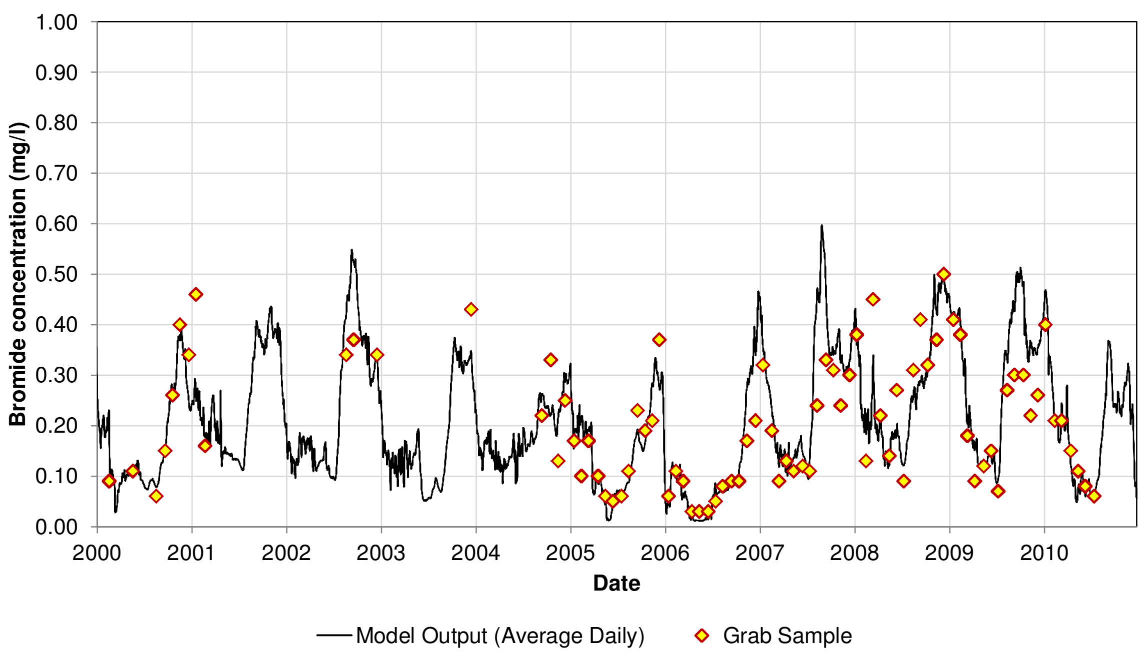

Figure 24b. Comparison Grab Sample Data and Simulated Daily Average Bromide Concentration at Banks Pumping Plant

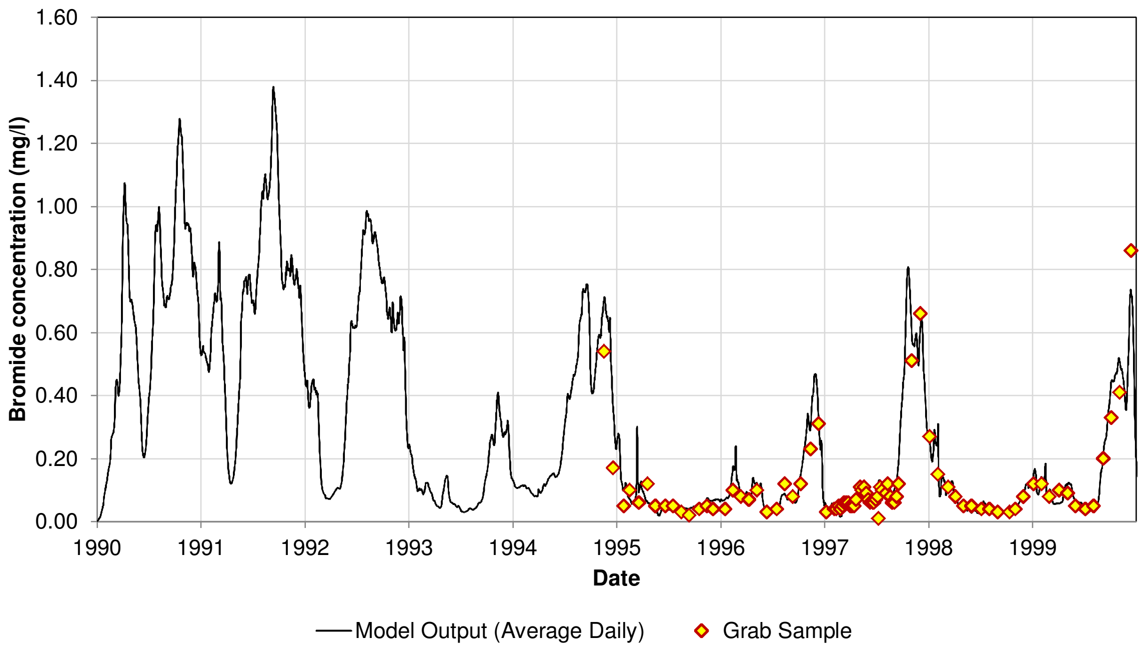

Figure 25a. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration in Old River at Bacon Island

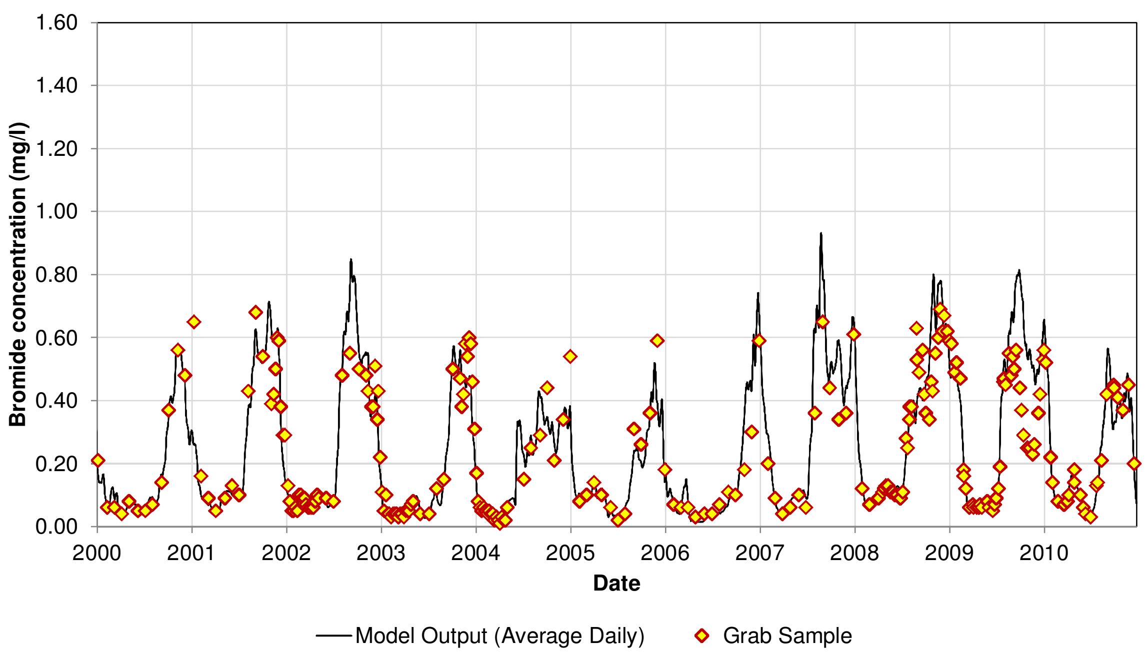

Figure 25b. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration in Old River at Bacon Island

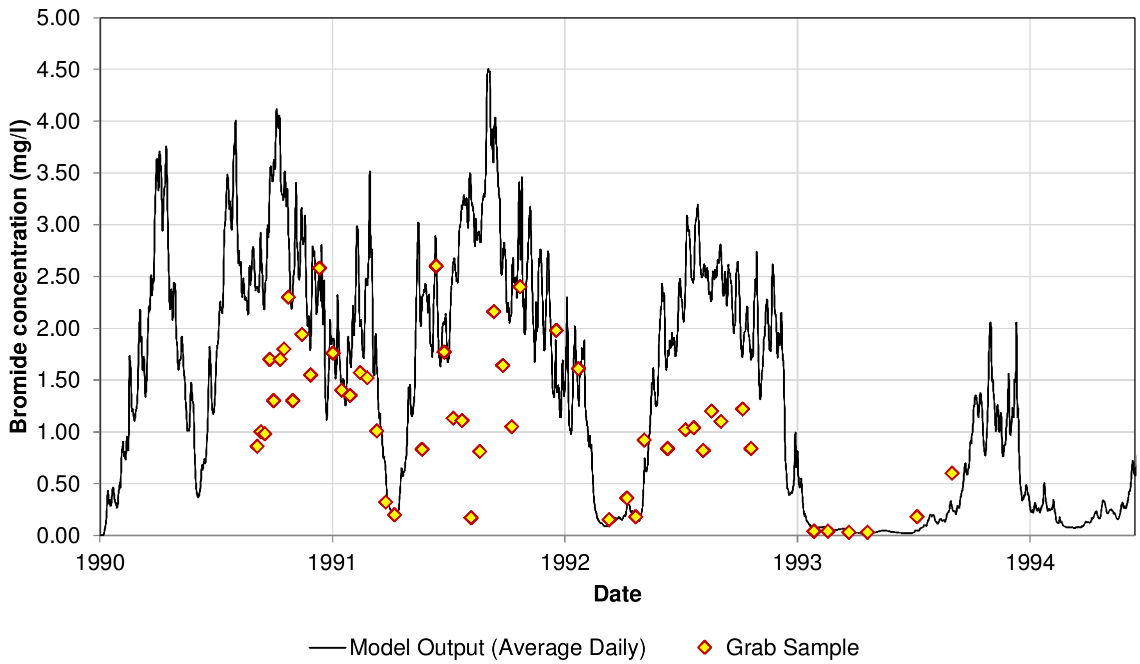

Figure 26. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration in San Joaquin River at Jersey Point

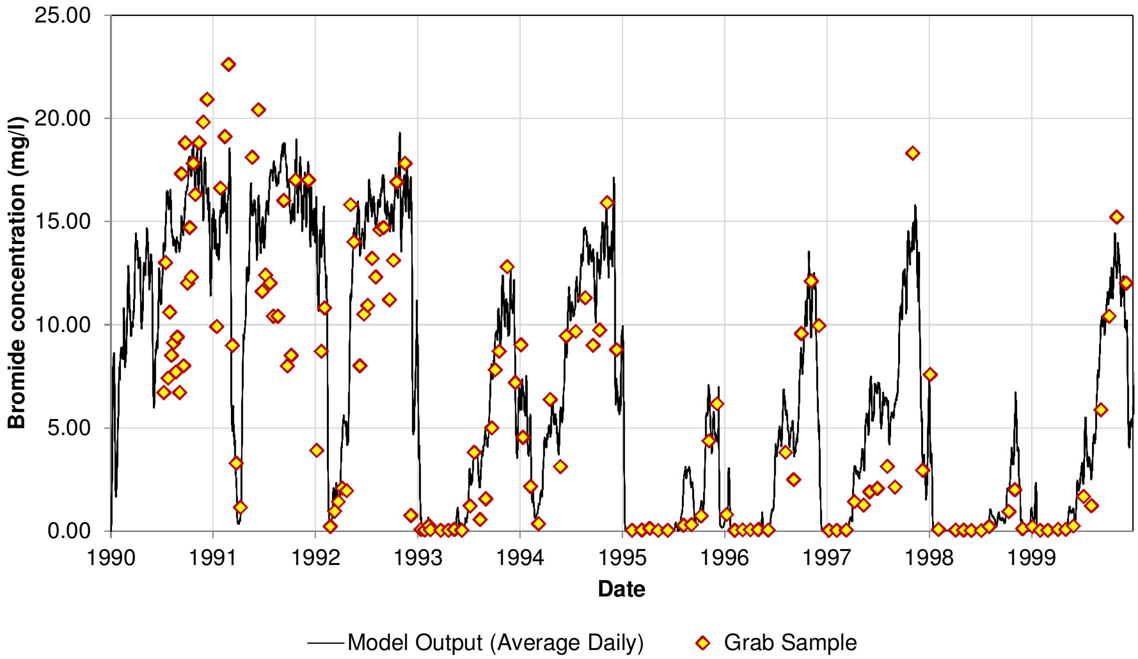

Figure 27a. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration in Sacramento River at Mallard Island

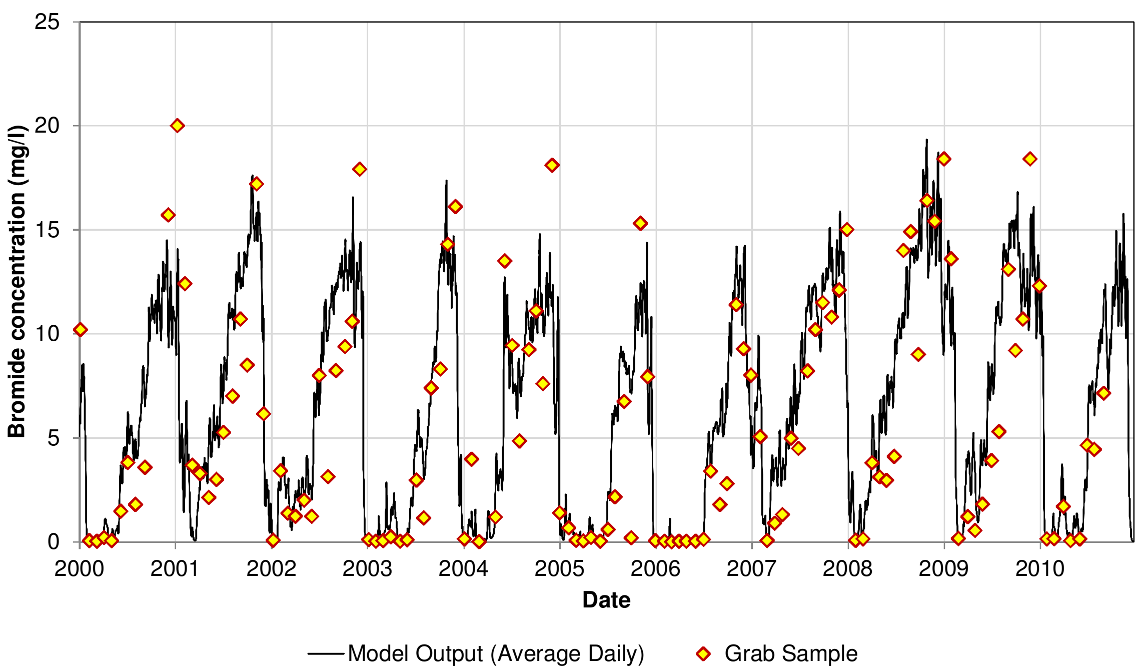

Figure 27b. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration in Sacramento River at Mallard Island

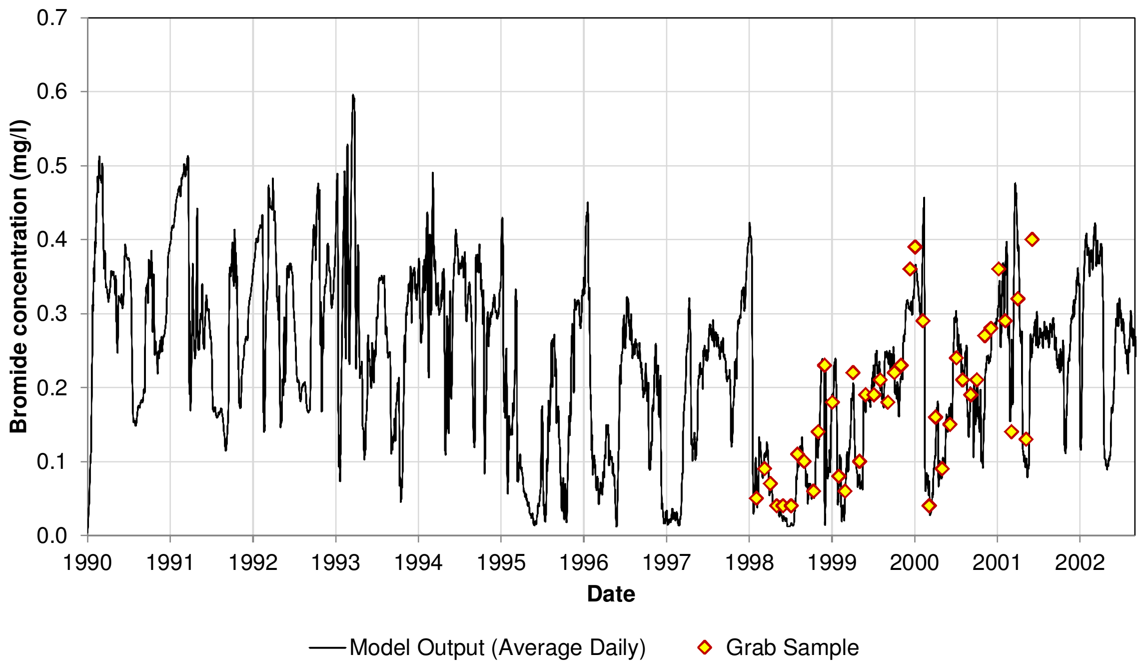

Figure 28. Comparison of Grab Sample Data and Simulated Daily Average Bromide Concentration in San Joaquin River at Highway 4

4.4 Sulfate

This section provides a summary of model performances in simulating sulfate concentrations at six Delta locations. Table 9 presents a summary of Bias, RMSE and NRMSE values for sulfate simulations at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that the DSM2 model simulates sulfate concentrations in the Delta reasonably well except in San Joaquin River at Jersey Point. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. It is noted that there were only few grab sample data for sulfate concentrations in San Joaquin River at Jersey Point compared to other locations. Average RMSE values show that the model performs well at matching the observed values. Average Bias values in Table 9 indicate that there is a general trend of overestimation of observed sulfate concentrations at the six locations in the Delta, which can be also seen in the scatter plots presented in Figure 29. Figures 30 through 35 show the time-series plots of grab sample data and simulated daily average sulfate concentrations at the six Delta locations. From Figures 30 through 35, it can be seen that the model outputs follow the trend in observed data reasonably well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating sulfate concentration at lower salinity levels than at higher salinity levels.

Table 9. Validation Summary Statistics for Sulfate Simulation at Different Locations in the Delta

Locations	Average Sulfate Concentration		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	48.35	44.75	3.60	29.28	25%	101
Banks Pumping Plant	36.45	36.50	-0.04	16.72	12%	152
Old River at Bacon Island	23.17	22.70	0.47	4.86	8%	215
San Joaquin River at Jersey Point	59.45	94.11	-34.66	50.42	68%	11
Sacramento River at Mallard Island	234.84	248.08	-14.25	79.20	9%	233
San Joaquin River at Highway 4	61.05	58.24	2.81	11.06	10%	41

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error
µS/cm = micro Siemens per centimeter

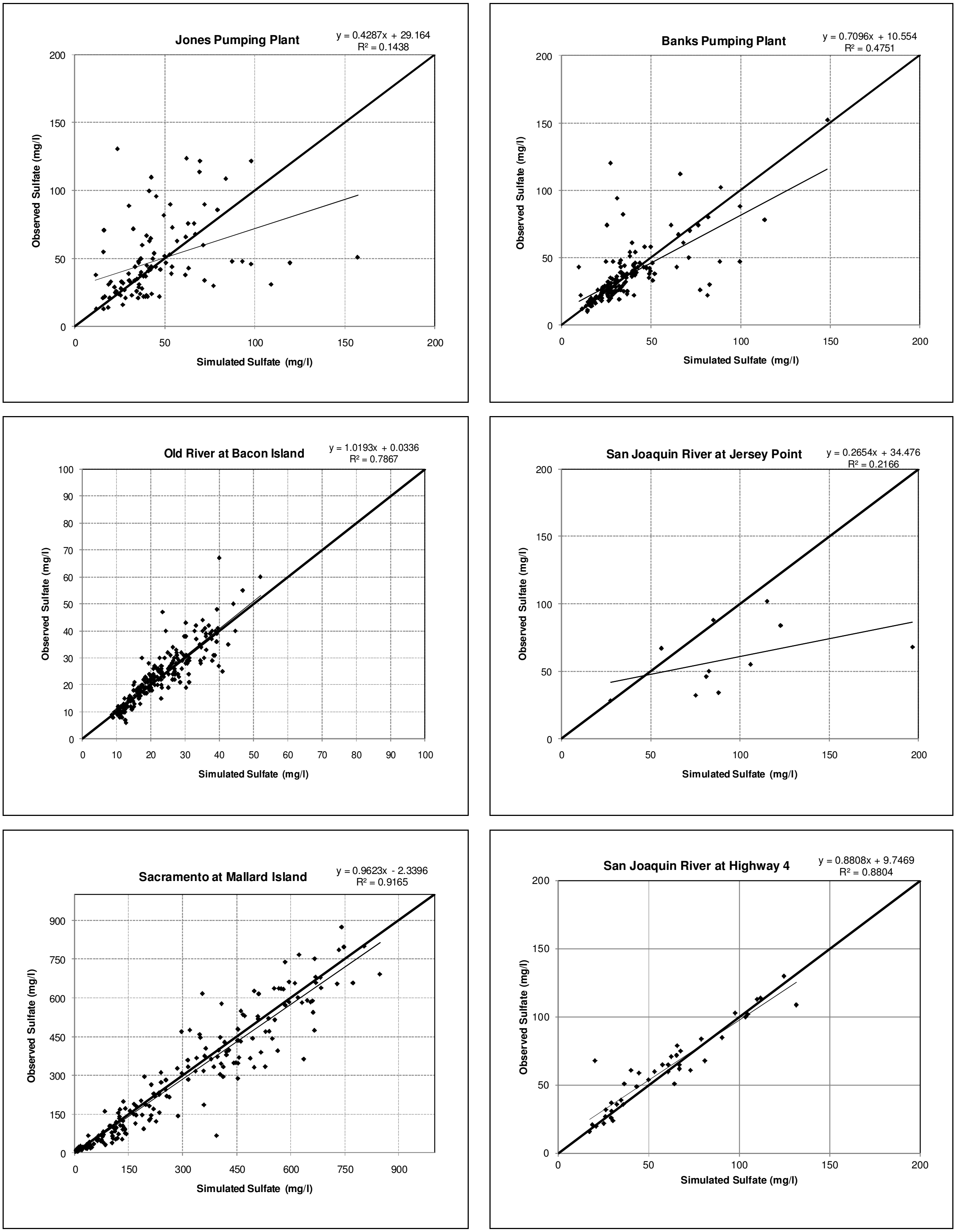

Figure 29. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

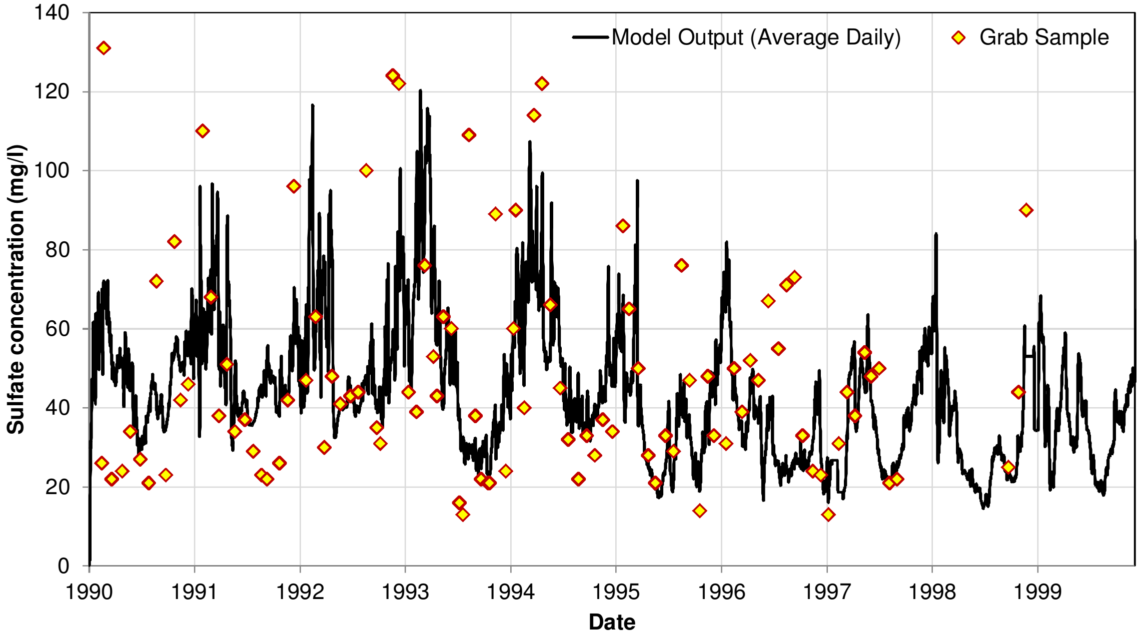

Figure 30. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration at Jones Pumping Plant

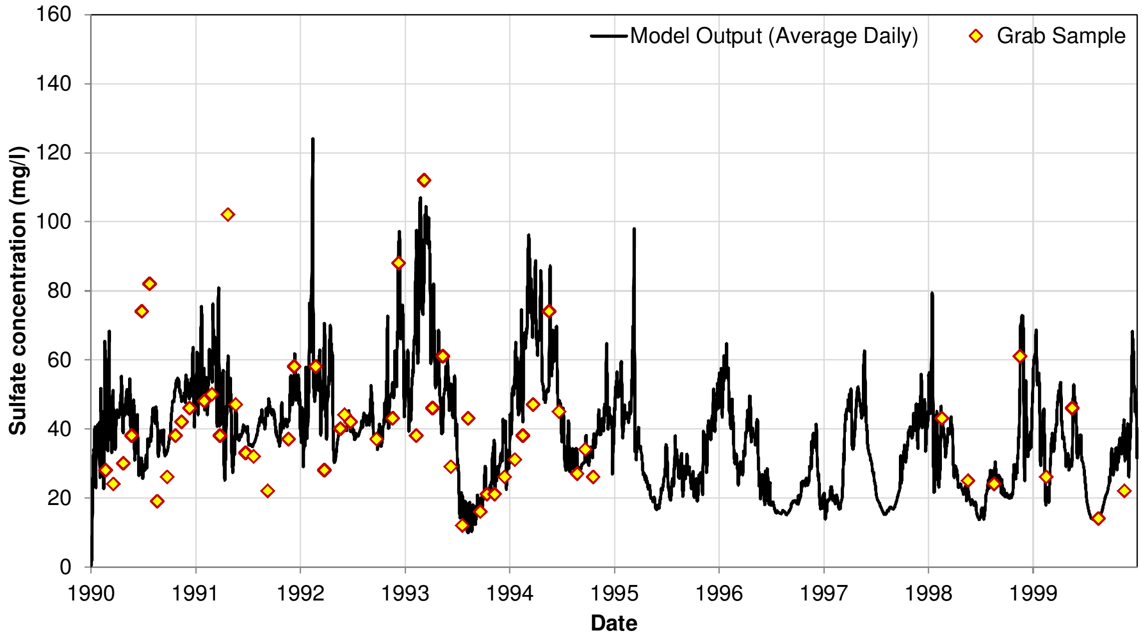

Figure 31a. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration at Banks Pumping Plant

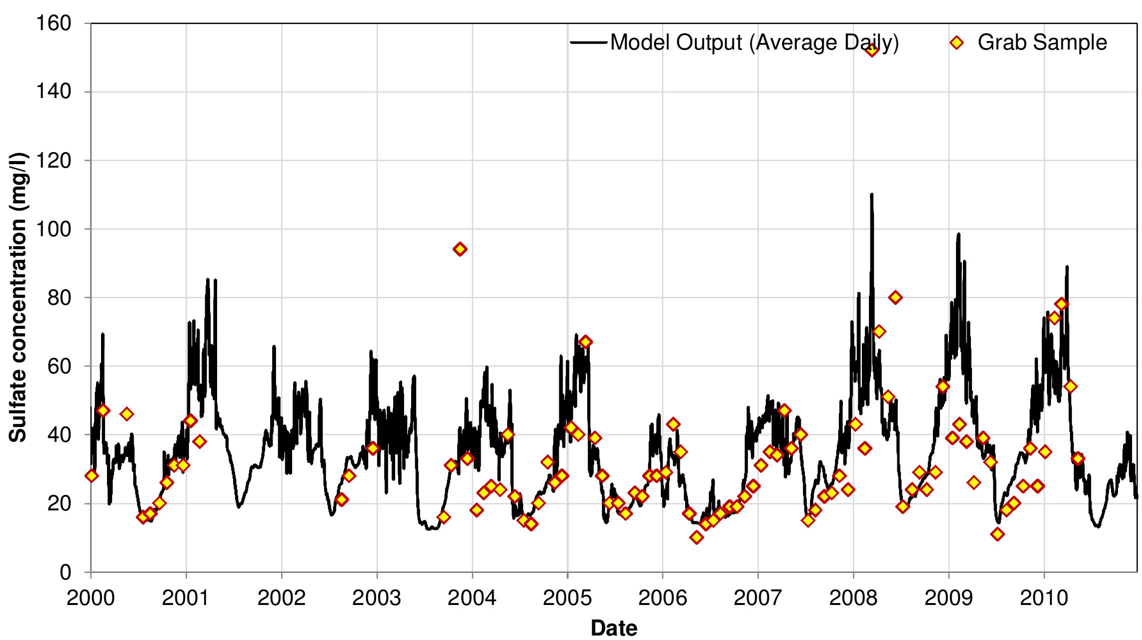

Figure 31b. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration at Banks Pumping Plant

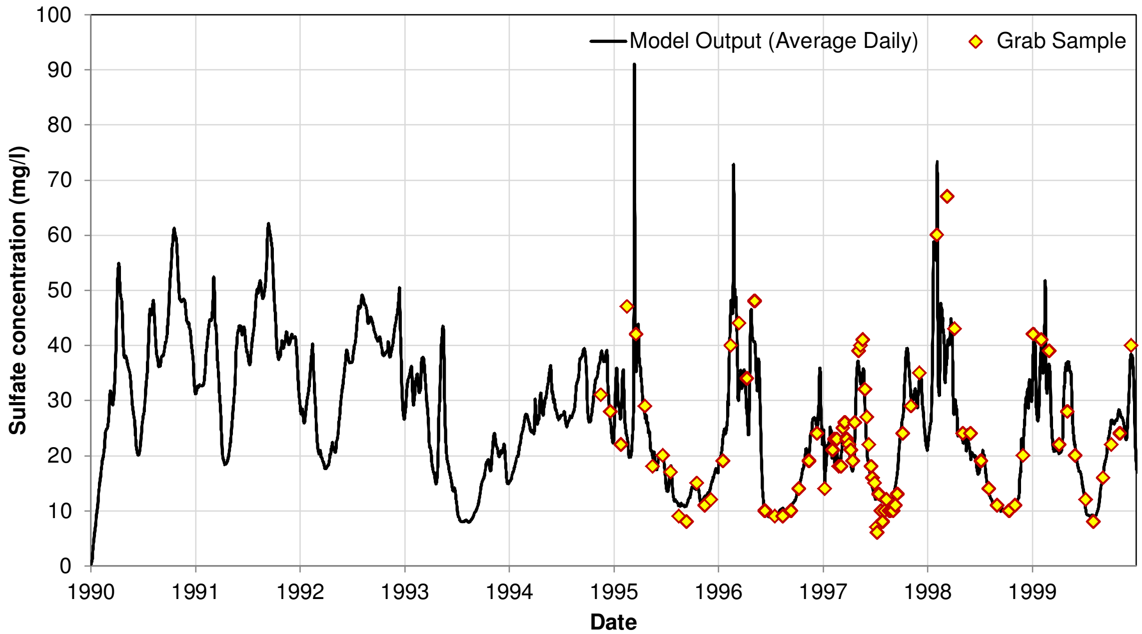

Figure 32a. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration in Old River at Bacon Island

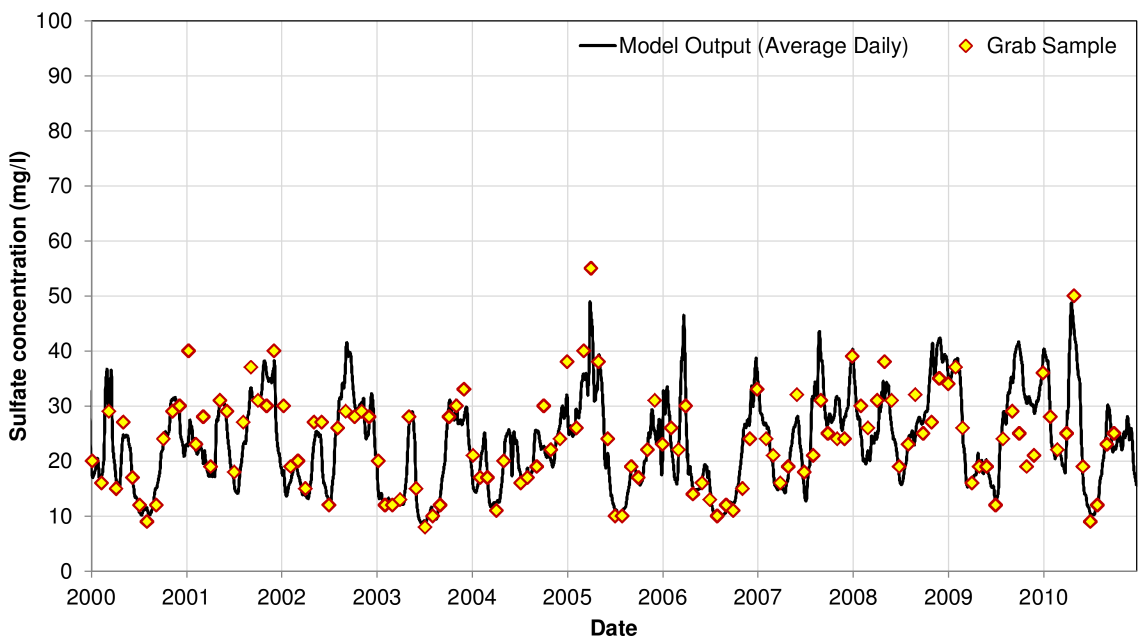

Figure 32b. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration in Old River at Bacon Island

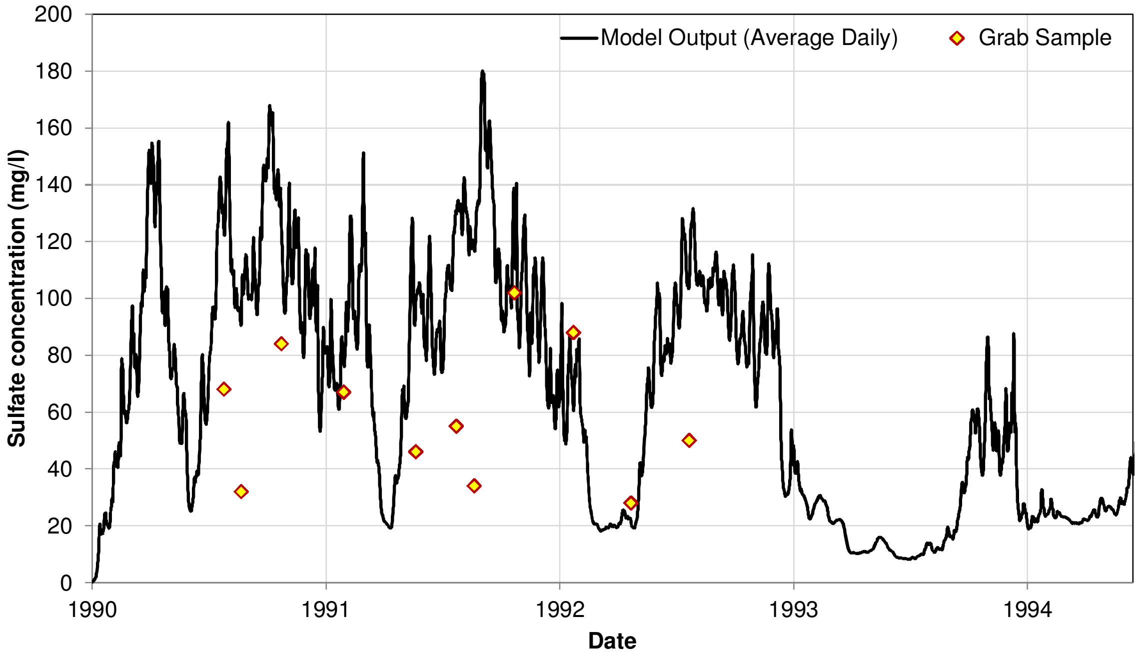

Figure 33. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration in San Joaquin River at Jersey Point

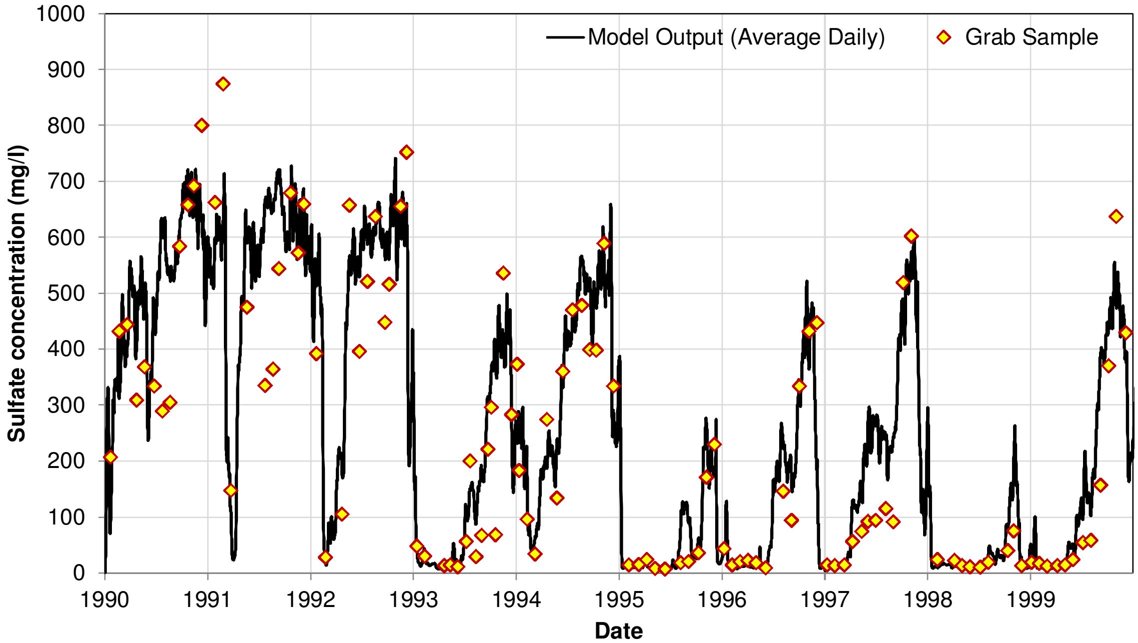

Figure 34a. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration in Sacramento River at Mallard Island

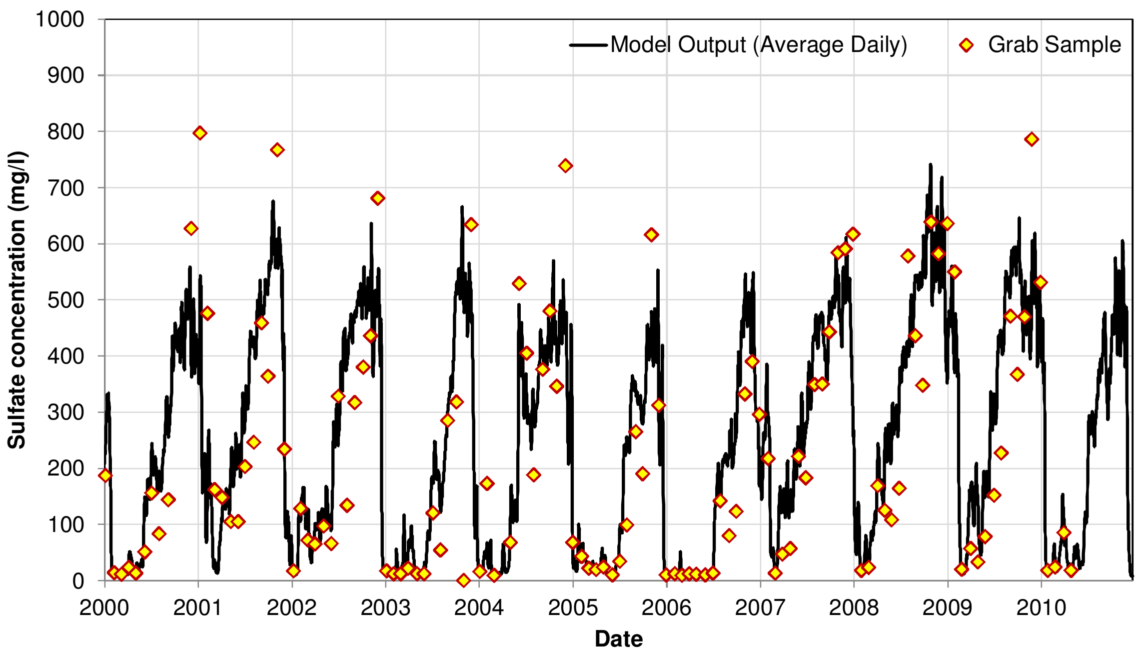

Figure 34b. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration in Sacramento River at Mallard Island

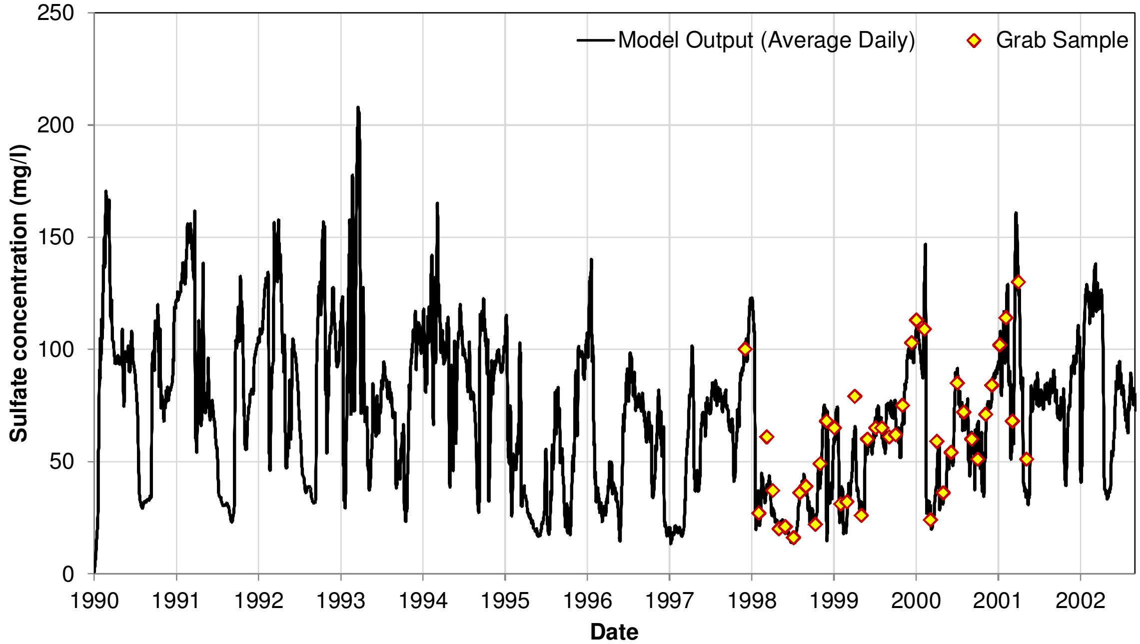

Figure 35. Comparison of Grab Sample Data and Simulated Daily Average Sulfate Concentration in San Joaquin River at Highway 4

4.5 Calcium

This section provides a summary of model performances in simulating calcium concentrations at six Delta locations. Table 10 presents a summary of Bias, RMSE and NRMSE values for calcium at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that DSM2 simulates calcium concentrations in the Delta reasonably well. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. Average Bias values in Table 10 indicate that there is a general trend of overestimation of observed calcium concentrations at the six locations in the Delta which can be also seen in the scatter plots presented in Figure 36. Figure 37 through 42 show the time-series plots of grab sample data and simulated daily average calcium concentrations. From Figures 37 through 42, it can be seen that the model outputs follow the trend in observed data reasonably well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating calcium concentration at lower salinity levels than at higher salinity levels.

Table 10. Validation Summary Statistics for Calcium Simulation at Different Locations in the Delta

Locations	Average Calcium Concentration		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	23.87	22.70	1.17	9.65	22%	135
Banks Pumping Plant	19.09	19.92	-0.83	4.34	11%	152
Old River at Bacon Island	14.82	15.00	-0.18	1.77	11%	216
San Joaquin River at Jersey Point	20.88	23.99	-3.11	7.28	19%	51
Sacramento River at Mallard Island	50.31	53.76	-3.45	14.75	6%	273
San Joaquin River at Highway 4	25.08	24.30	0.77	4.94	15%	41

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

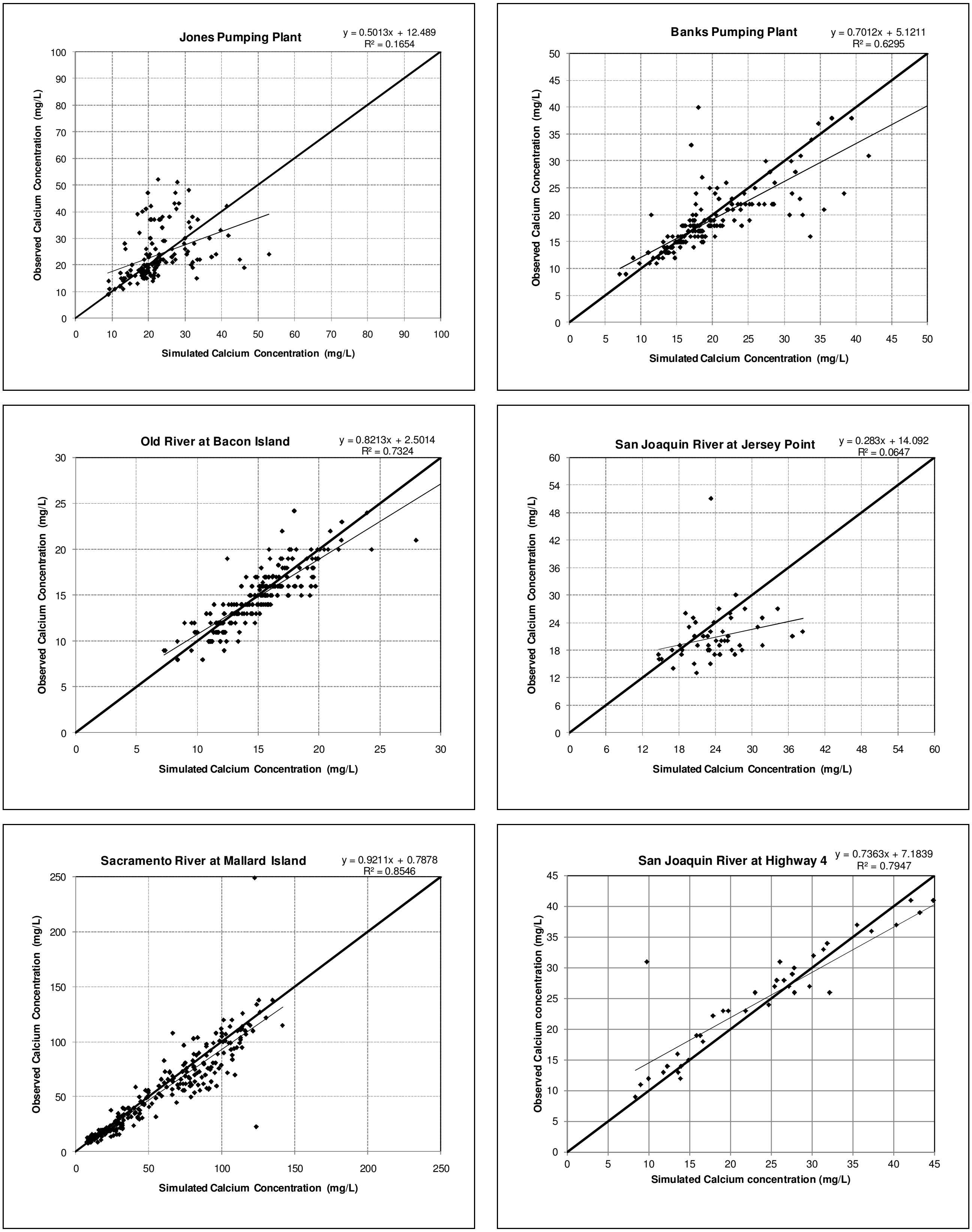

Figure 36. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

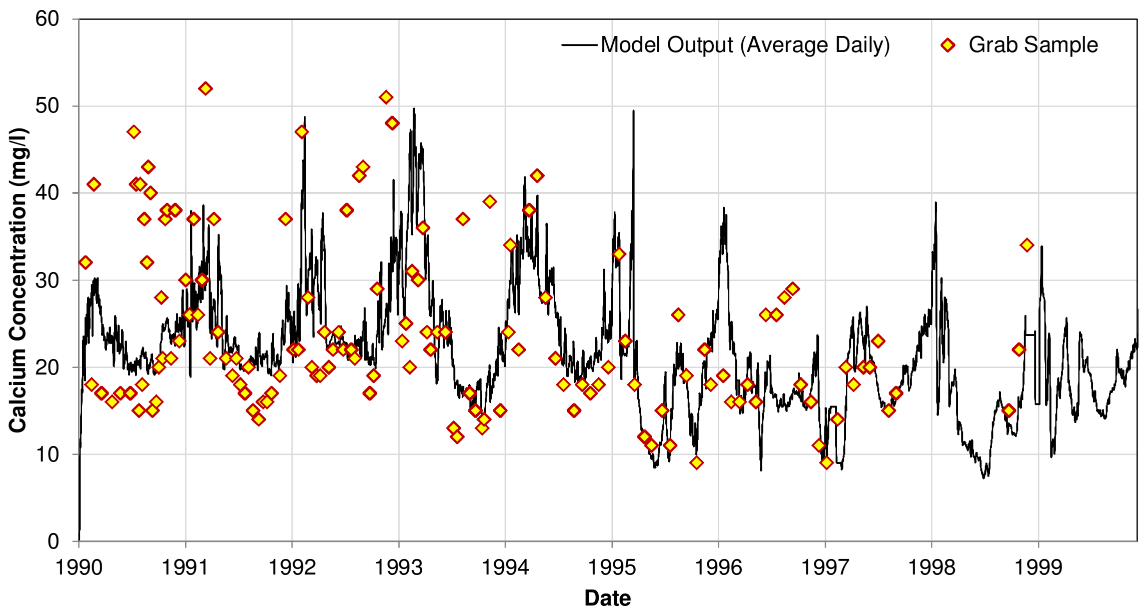

Figure 37. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration at Jones Pumping Plant

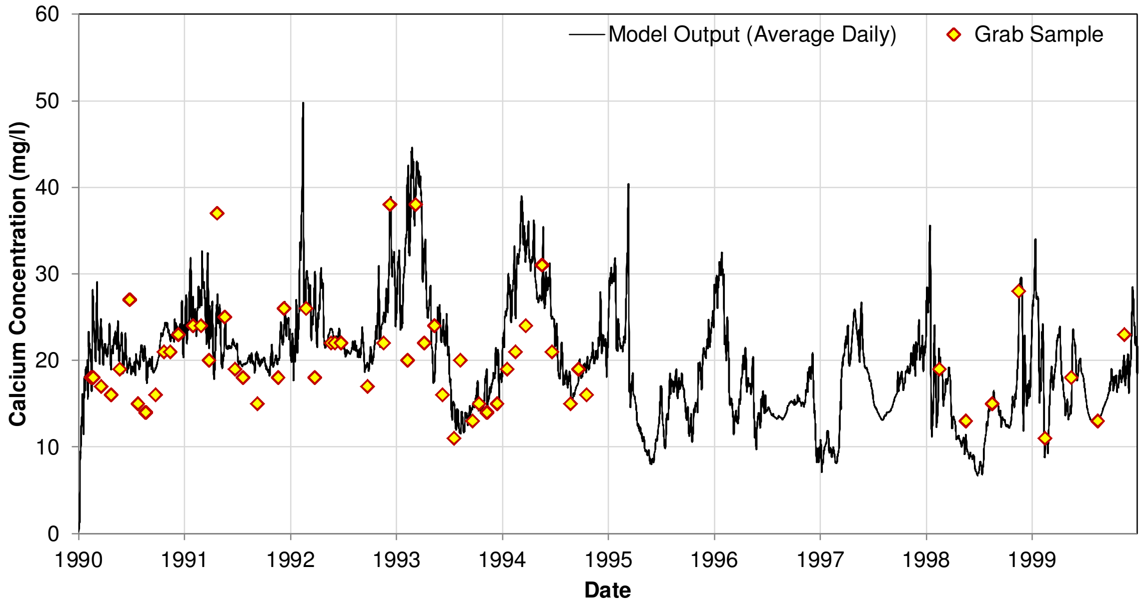

Figure 38a. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration at Banks Pumping Plant

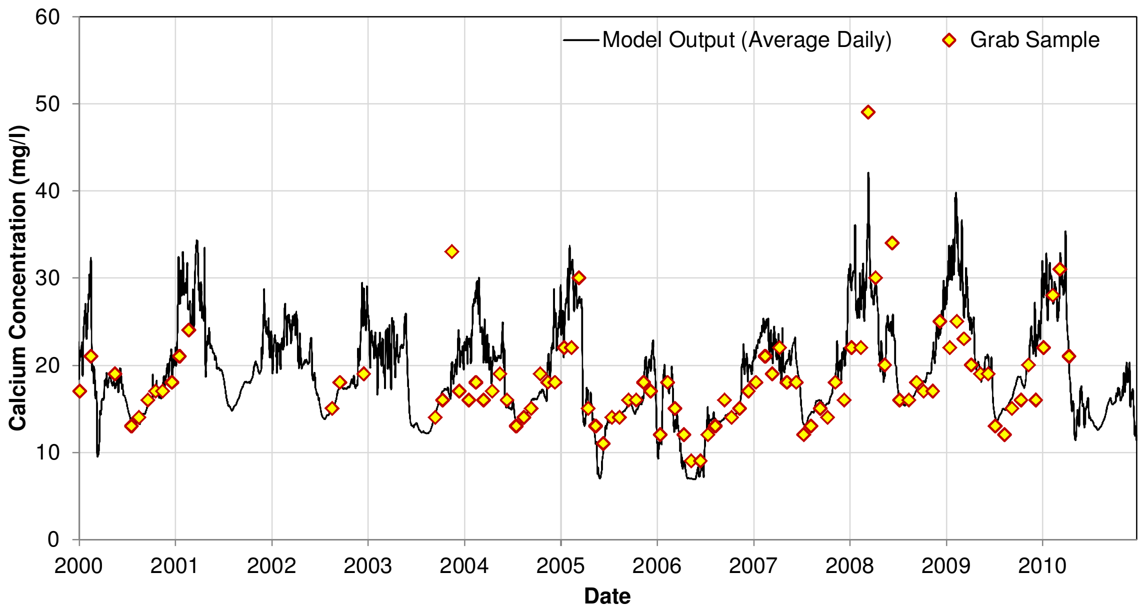

Figure 38b. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration at Banks Pumping Plant

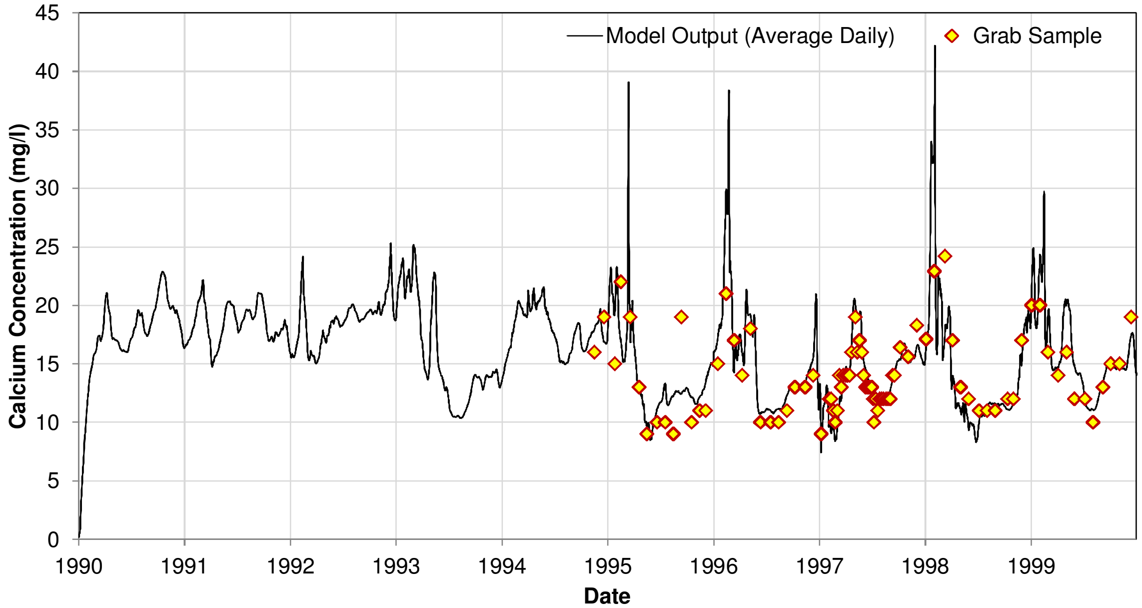

Figure 39a. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration in Old River at Bacon Island

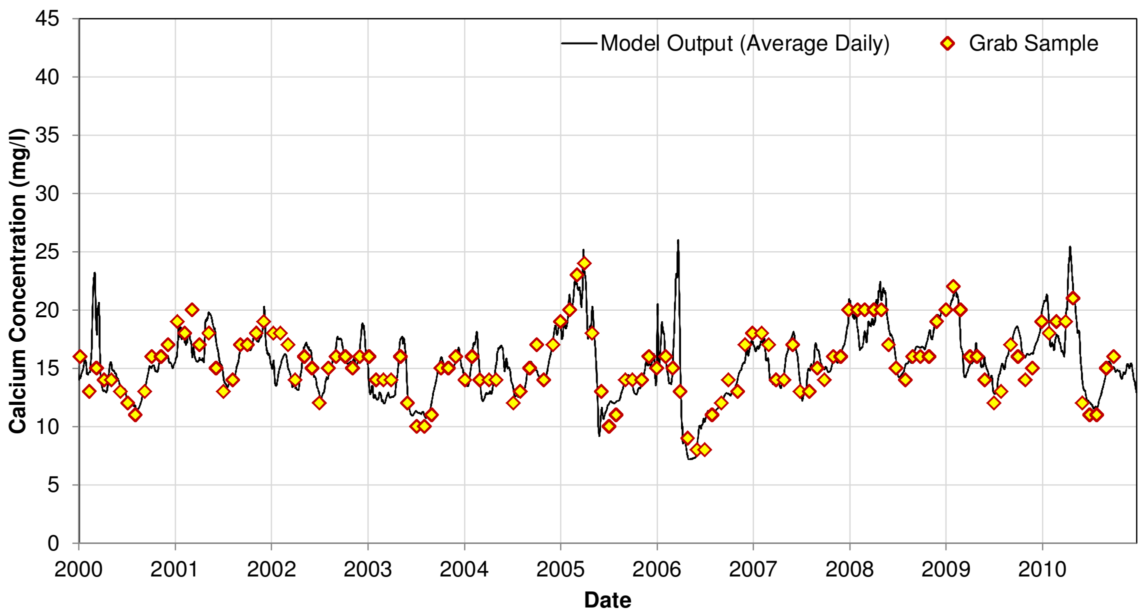

Figure 39b. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration in Old River at Bacon Island

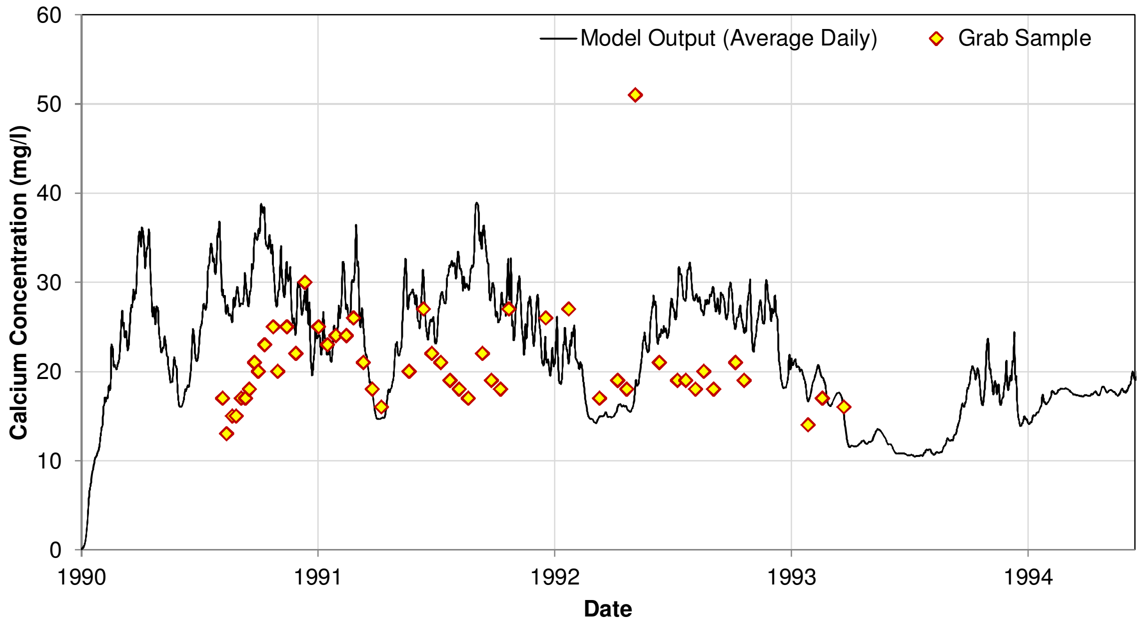

Figure 40. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration in San Joaquin River at Jersey Point

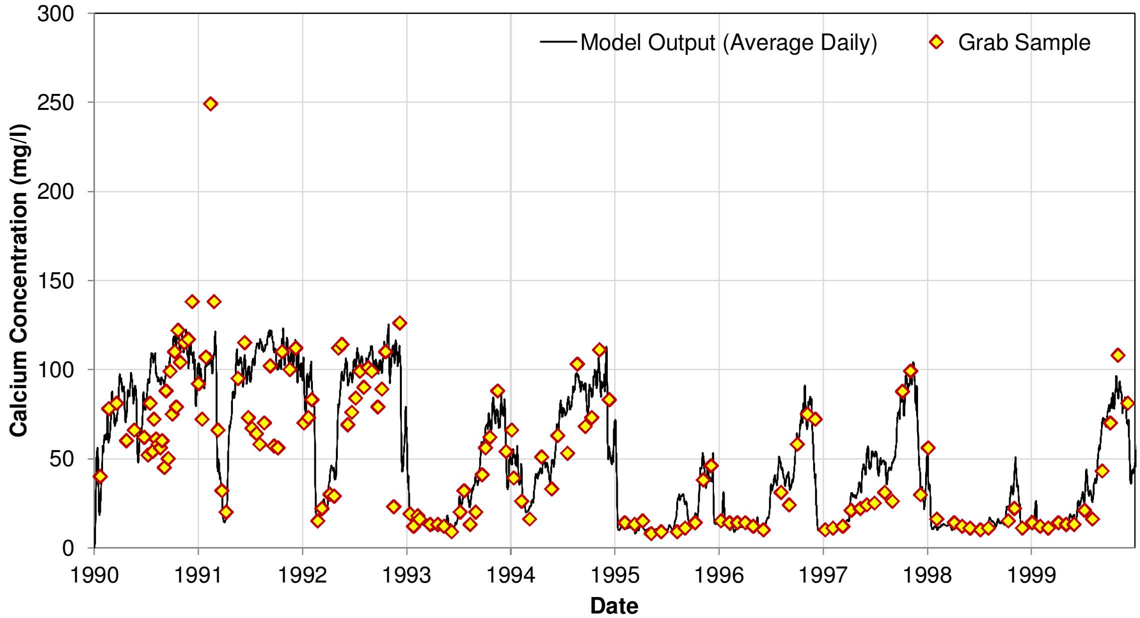

Figure 41a. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration in Sacramento River at Mallard Island

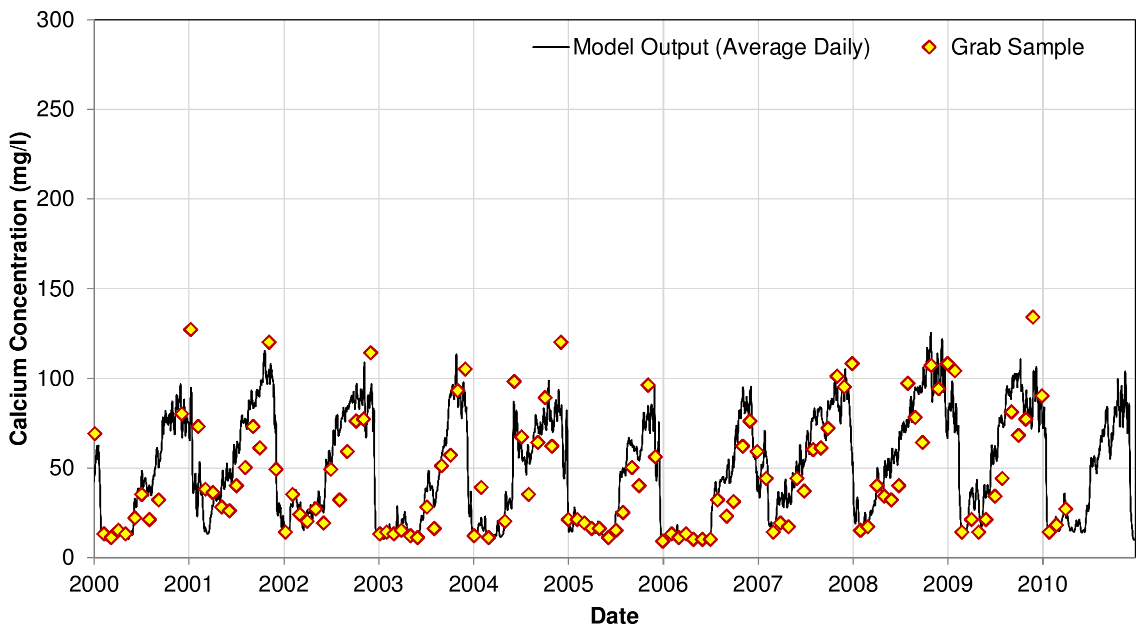

Figure 41b. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration in Sacramento River at Mallard Island

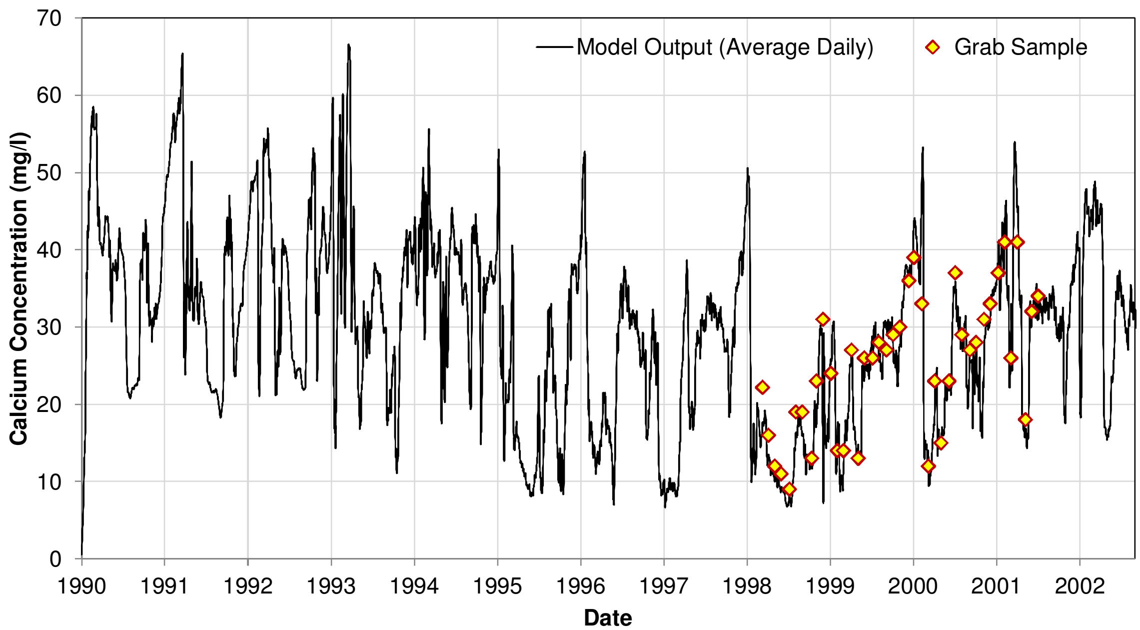

Figure 42. Comparison of Grab Sample Data and Simulated Daily Average Calcium Concentration in San Joaquin River at Highway 4

4.6 Magnesium

This section provides a summary of model performances in simulating magnesium concentrations at six Delta locations. Table 11 presents a summary of Bias, RMSE and NRMSE values for magnesium simulations at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that the DSM2 model simulates magnesium concentrations in the Delta reasonably well except in San Joaquin River at Jersey Point. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. Average Bias values in Table 11 indicate that there is a general trend of overestimation of observed magnesium concentrations at the six locations in the Delta which can be also seen in the scatter plots presented in Figure 43. Figures 44 through 49 show the time-series plots of grab sample data and simulated daily average magnesium concentrations at the six Delta locations. From Figures 44 through 49, it can be seen that the model outputs follow the trend in observed data well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating magnesium concentration at lower salinity levels than at higher salinity levels.

Table 11. Validation Summary Statistics for Magnesium Simulation at Different Locations in the Delta

Locations	Average Magnesium Concentration		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	14.87	14.77	0.10	4.55	17%	138
Banks Pumping Plant	12.77	13.04	-0.27	2.52	10%	152
Old River at Bacon Island	10.26	10.41	-0.15	1.88	9%	216
San Joaquin River at Jersey Point	30.41	40.51	-10.10	19.36	25%	51
Sacramento River at Mallard Island	129.43	144.36	-14.93	37.35	8%	273
San Joaquin River at Highway 4	12.14	11.83	0.31	2.48	14%	38

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

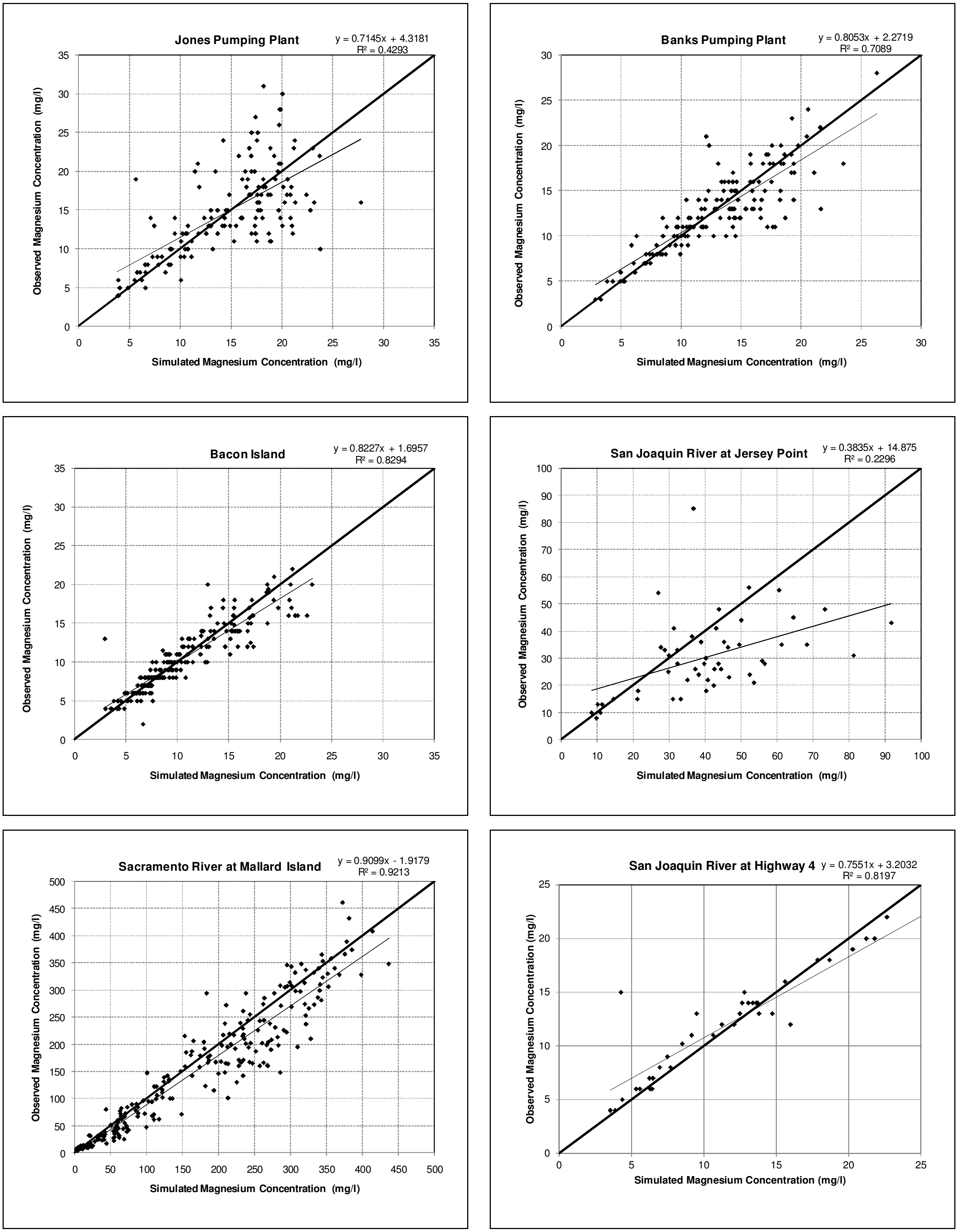

Figure 43. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

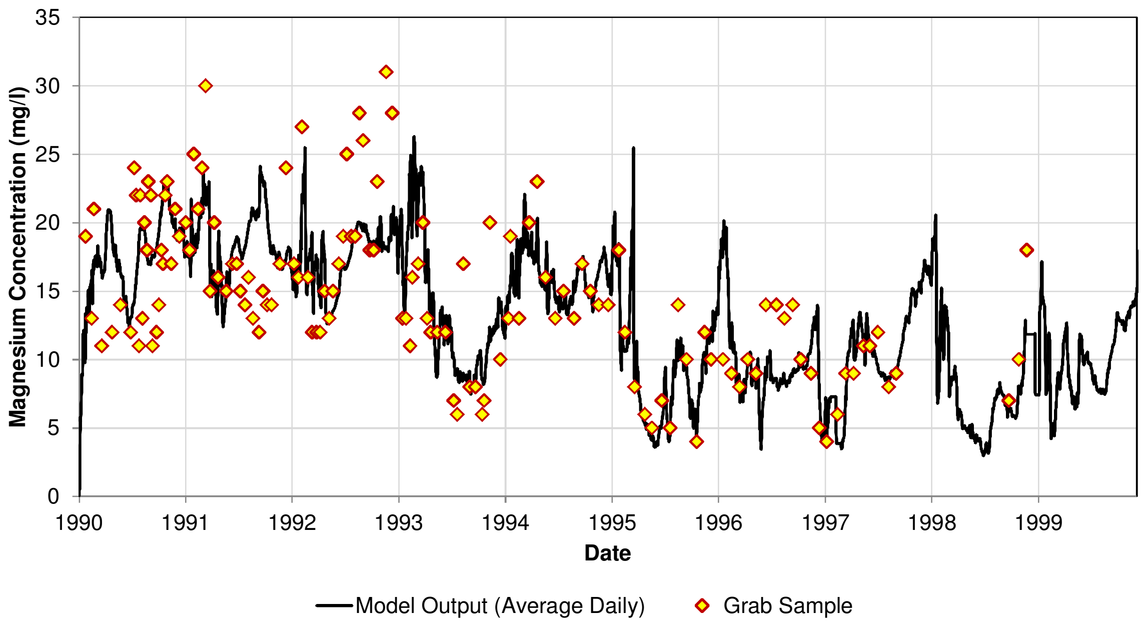

Figure 44. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration at Jones Pumping Plant

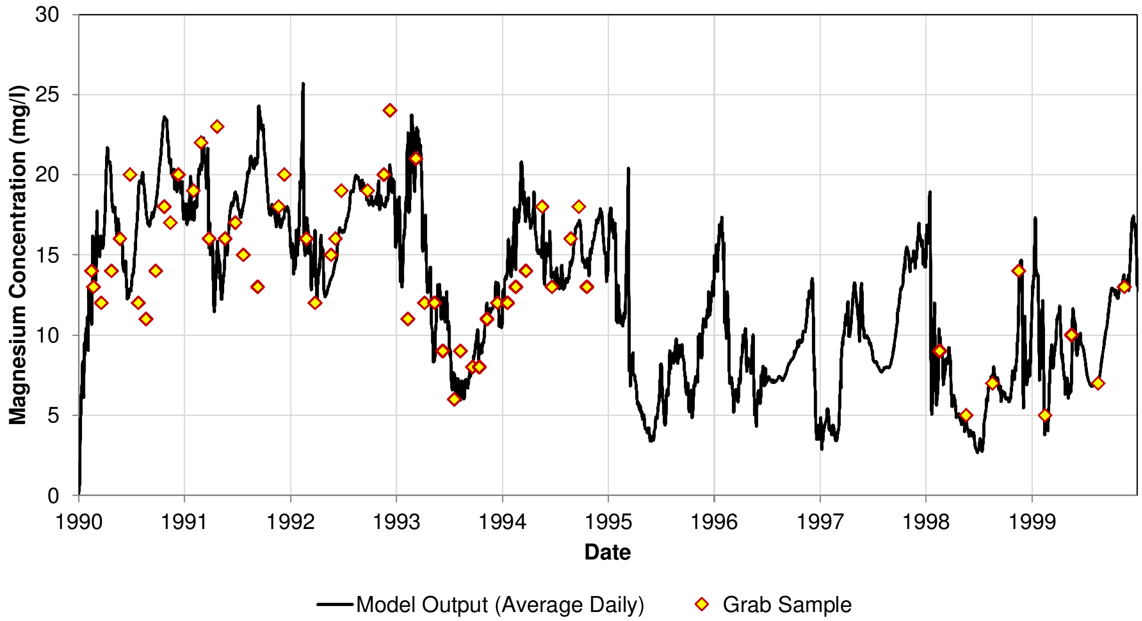

Figure 45a. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration at Banks Pumping Plant

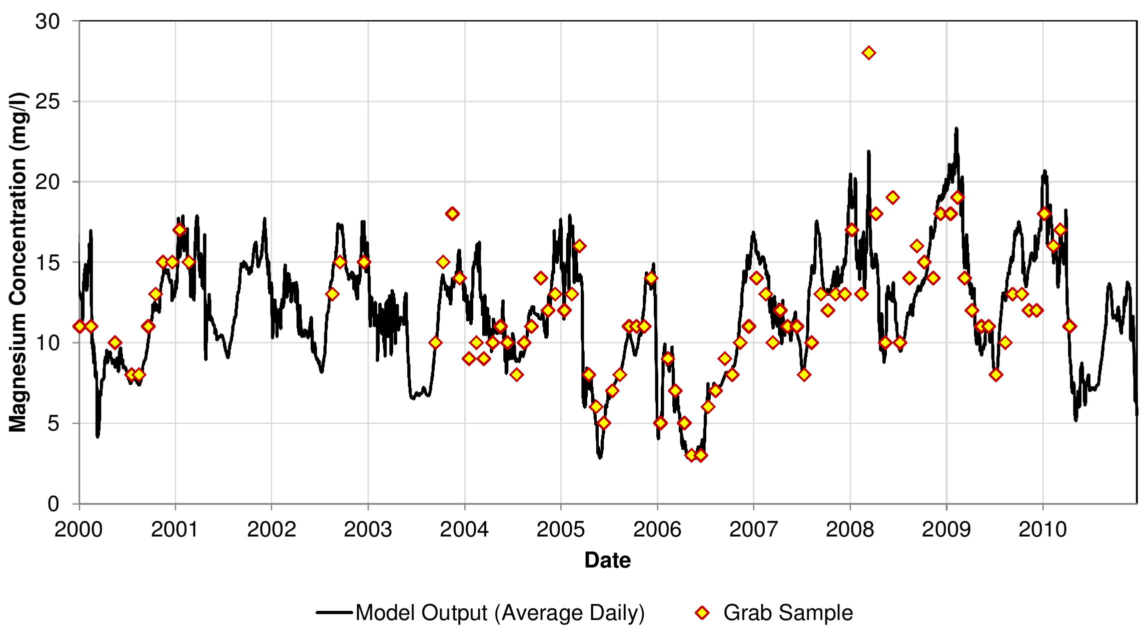

Figure 45b. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration at Banks Pumping Plant

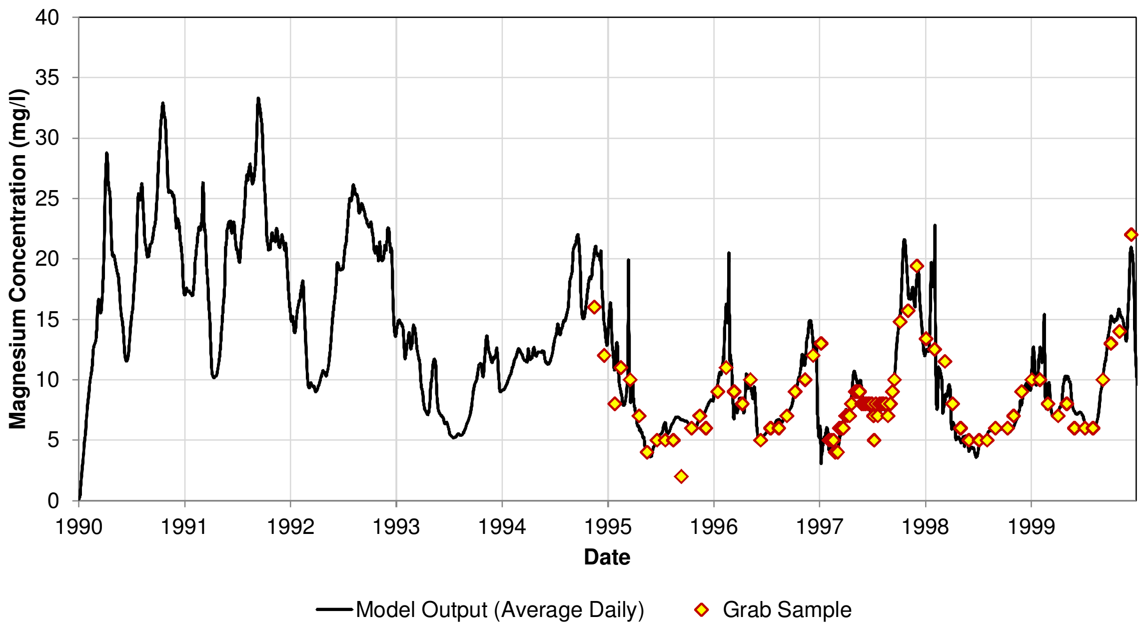

Figure 46a. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration at in Old River at Bacon Island

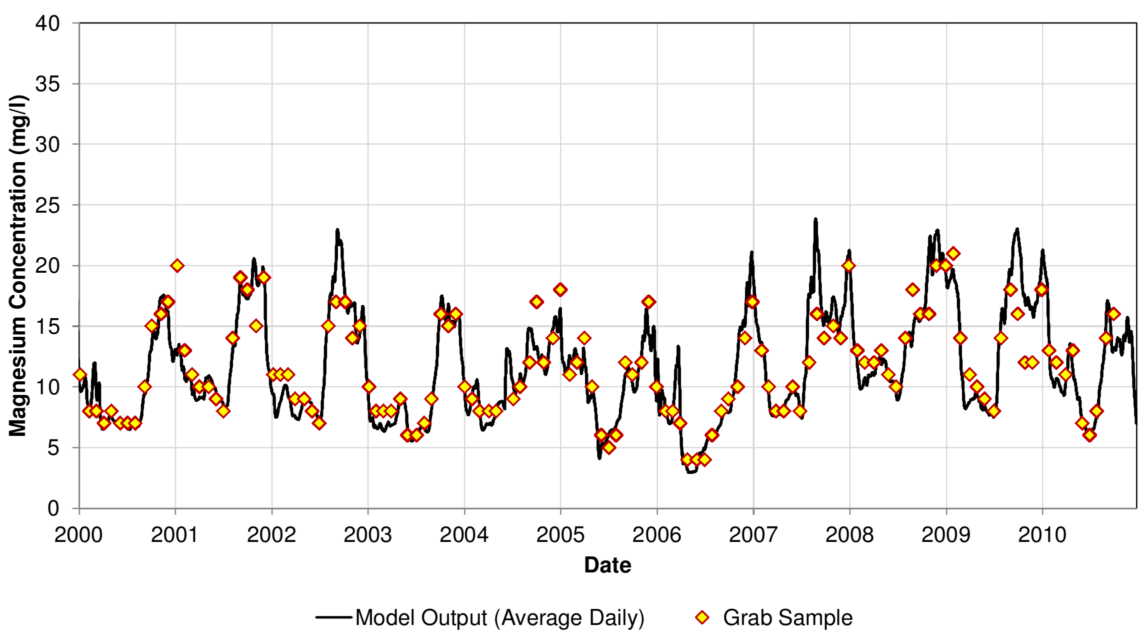

Figure 46b. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration at in Old River at Bacon Island

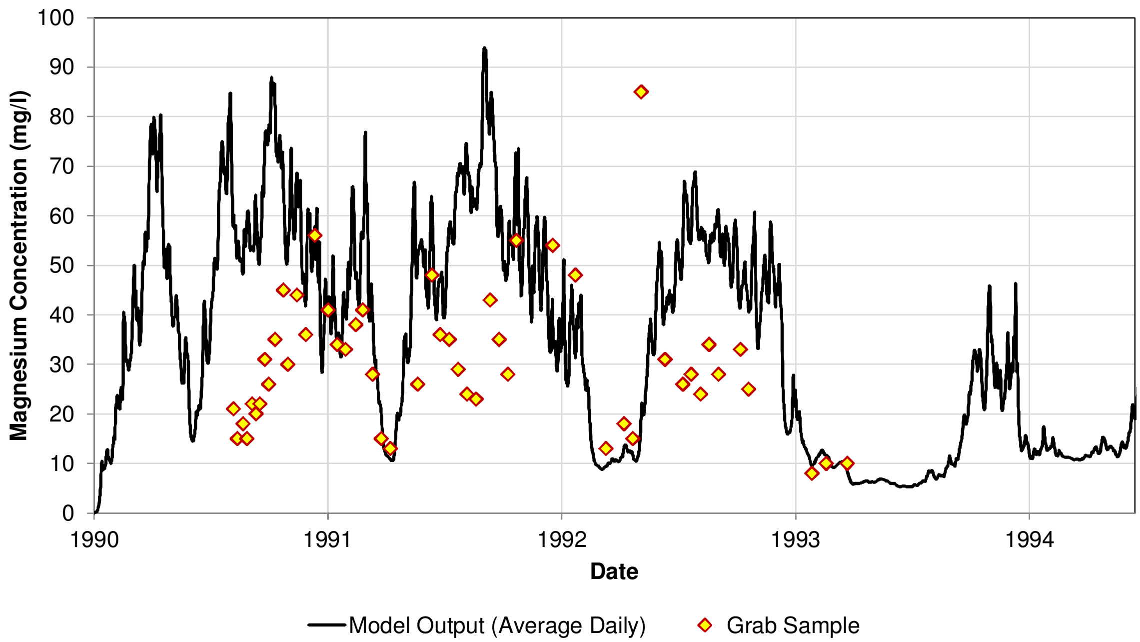

Figure 47. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration at in San Joaquin River at Jersey Point

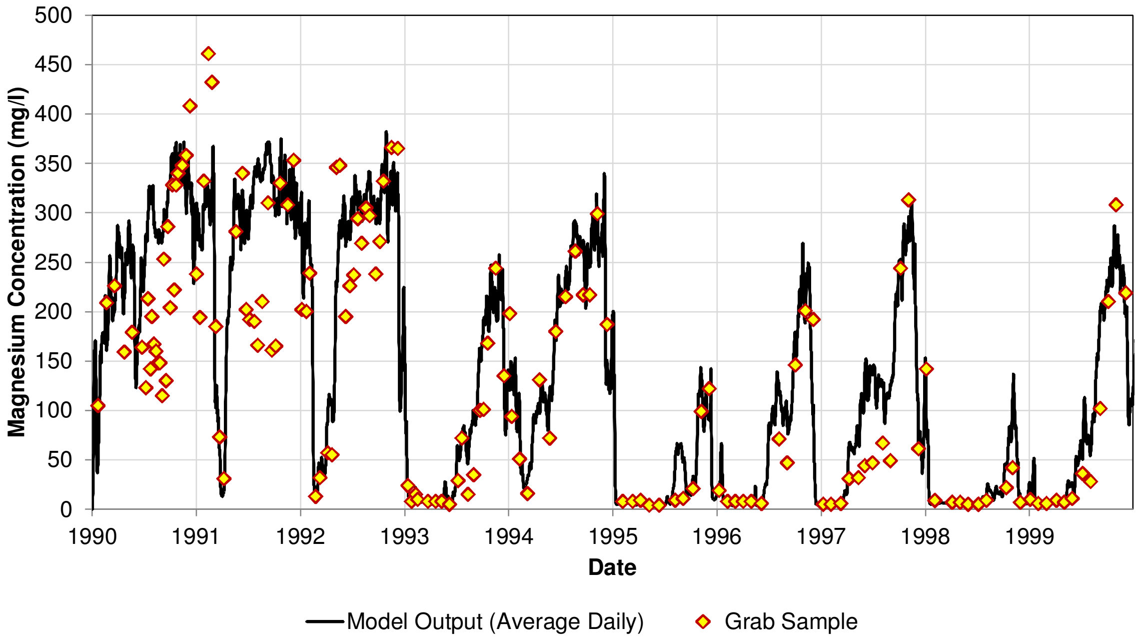

Figure 48a. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration in Sacramento River at Mallard Island

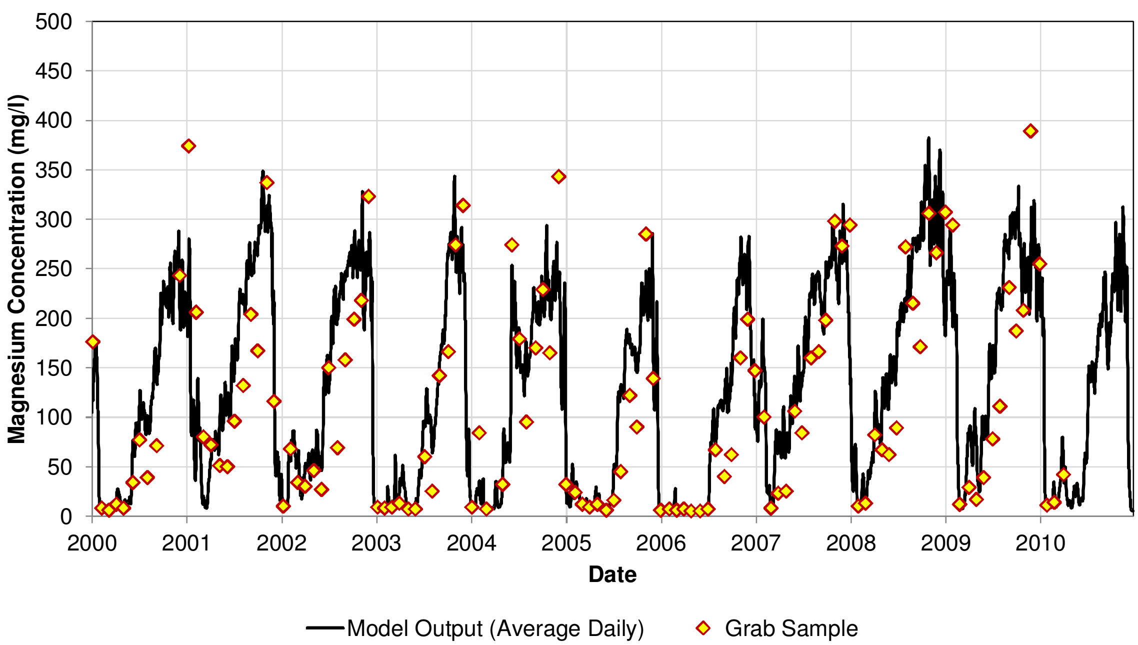

Figure 48b. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration in Sacramento River at Mallard Island

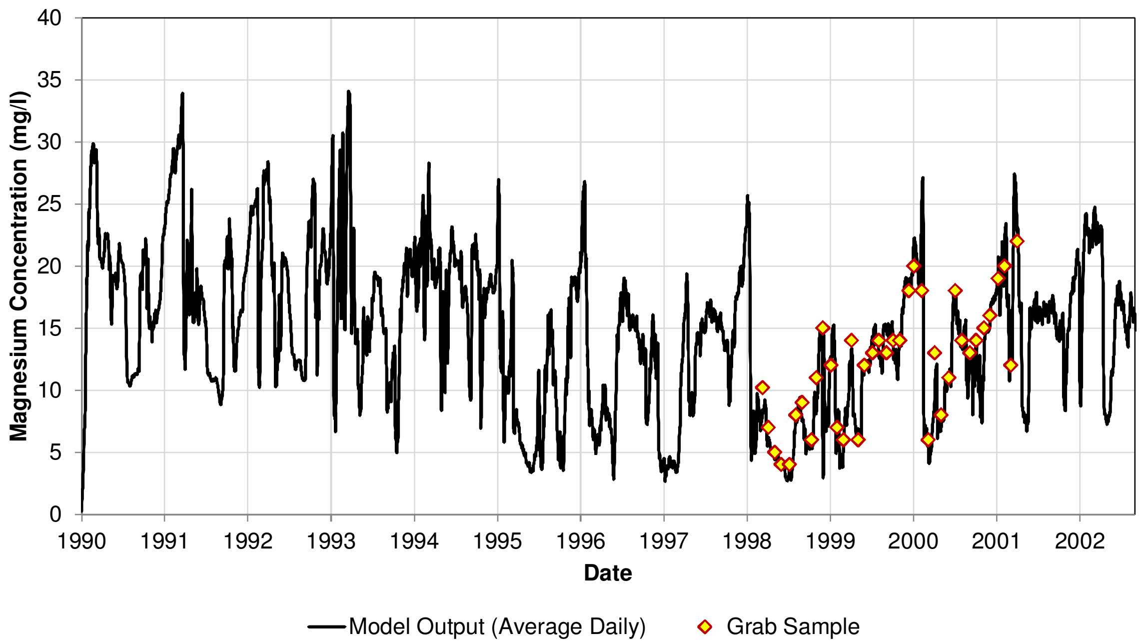

Figure 49. Comparison of Grab Sample Data and Simulated Daily Average Magnesium Concentration in San Joaquin River at Highway 4

4.7 Sodium

This section provides a summary of model performances in simulating sodium concentrations at six Delta locations. Table 12 presents a summary of Bias, RMSE and NRMSE values for sodium simulations at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that the DSM2 model simulates sodium concentrations in the Delta reasonably well except in San Joaquin River at Jersey Point. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. Average Bias values in Table 12 indicate that there is a general trend of overestimation of observed sodium concentrations at the six locations in the Delta which can be also seen in the scatter plots presented in Figure 50. Figures 51 through 56 show the time-series plots of grab sample data and simulated daily average sodium concentrations at the six Delta locations. From Figures 51 through 56, it can be seen that the model outputs follow the trend in observed data well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating sodium concentration at lower salinity levels than at higher salinity levels.

Table 12. Validation Summary Statistics for Sodium Simulation at Different Locations in the Delta

Locations	Average Sodium Concentration		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	59.9	62.9	-3.0	24.6	19%	135
Banks Pumping Plant	50.0	49.8	0.2	16.2	14%	154
Old River at Bacon Island	39.6	38.0	1.6	11.5	8%	216
San Joaquin River at Jersey Point	180.5	250.6	-70.1	131.5	32%	51
Sacramento River at Mallard Island	1000.6	1076.5	-75.9	276.0	8%	275
San Joaquin River at Highway 4	49.2	45.42	3.77	11.28	13%	31

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

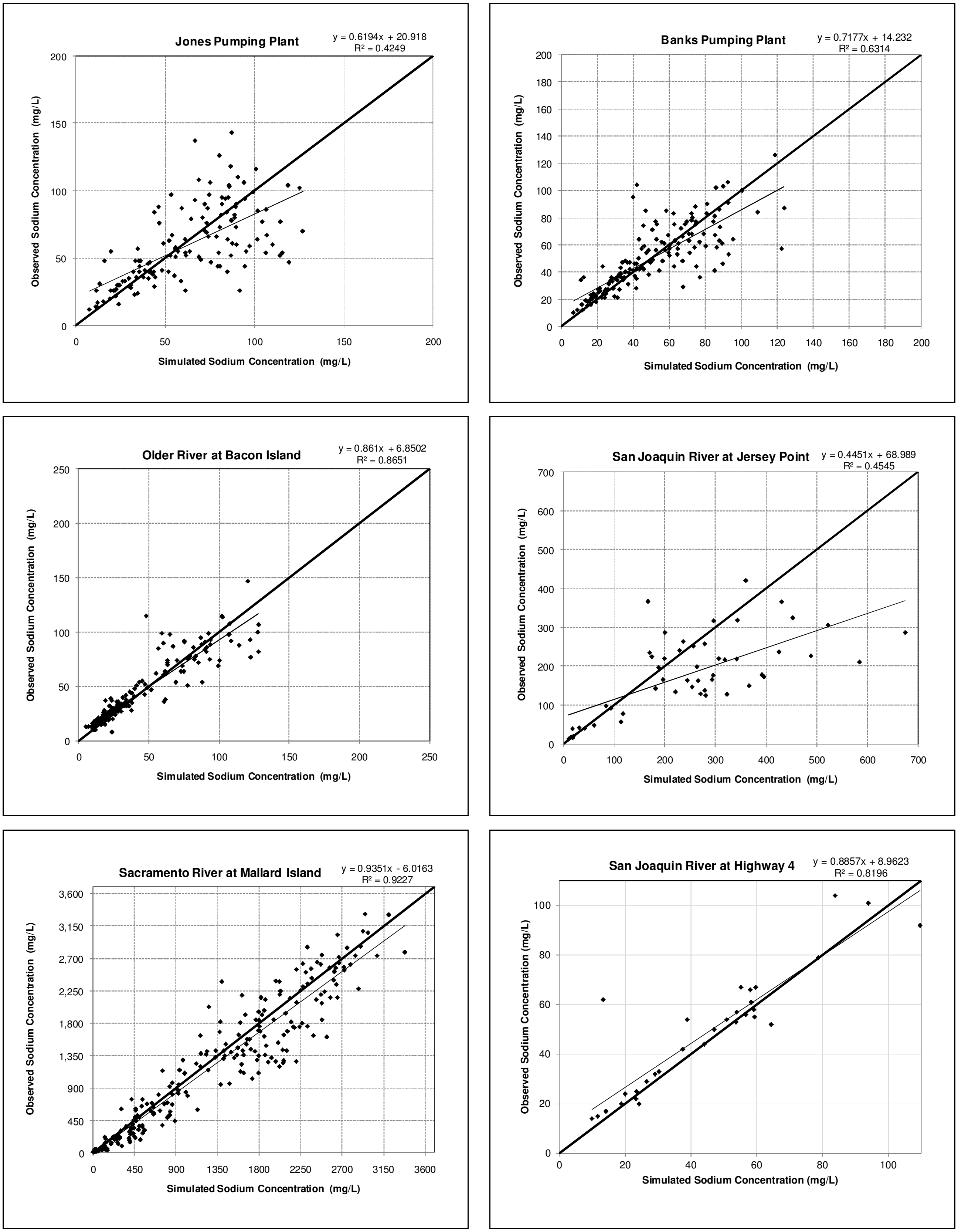

Figure 50. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

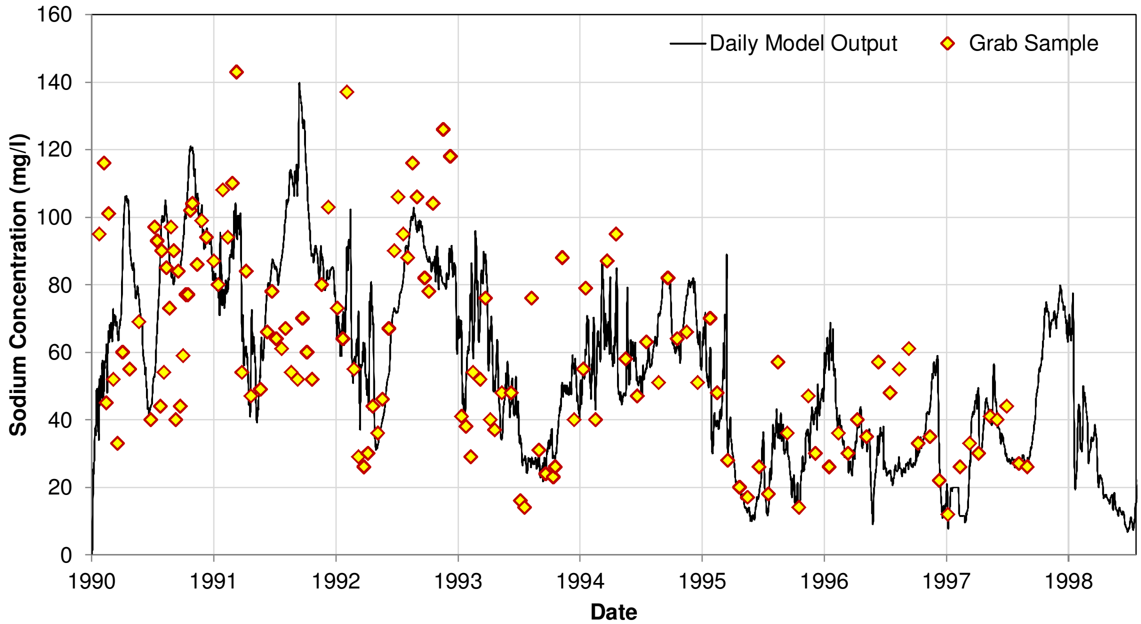

Figure 51. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration at Jones Pumping Plant

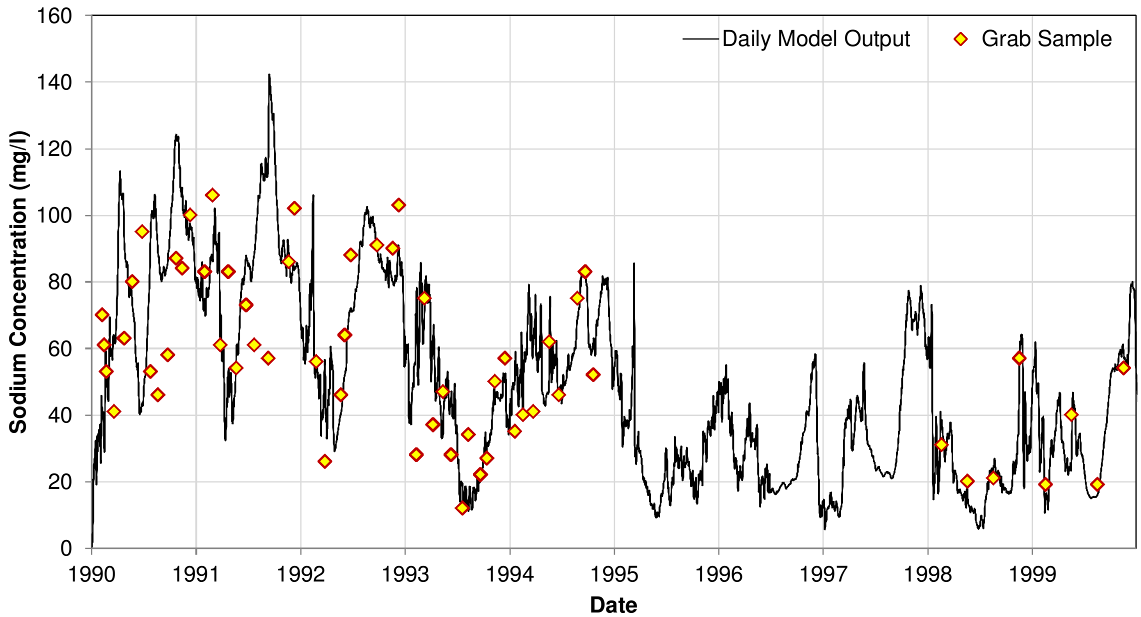

Figure 52a. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration at Banks Pumping Plant

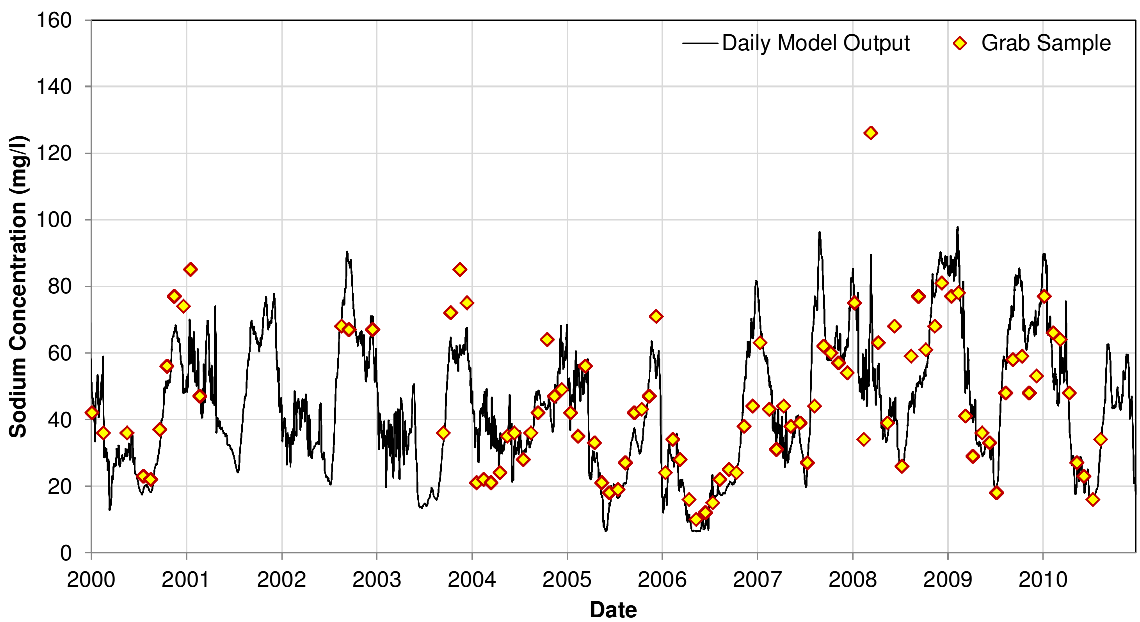

Figure 52b. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration at Banks Pumping Plant

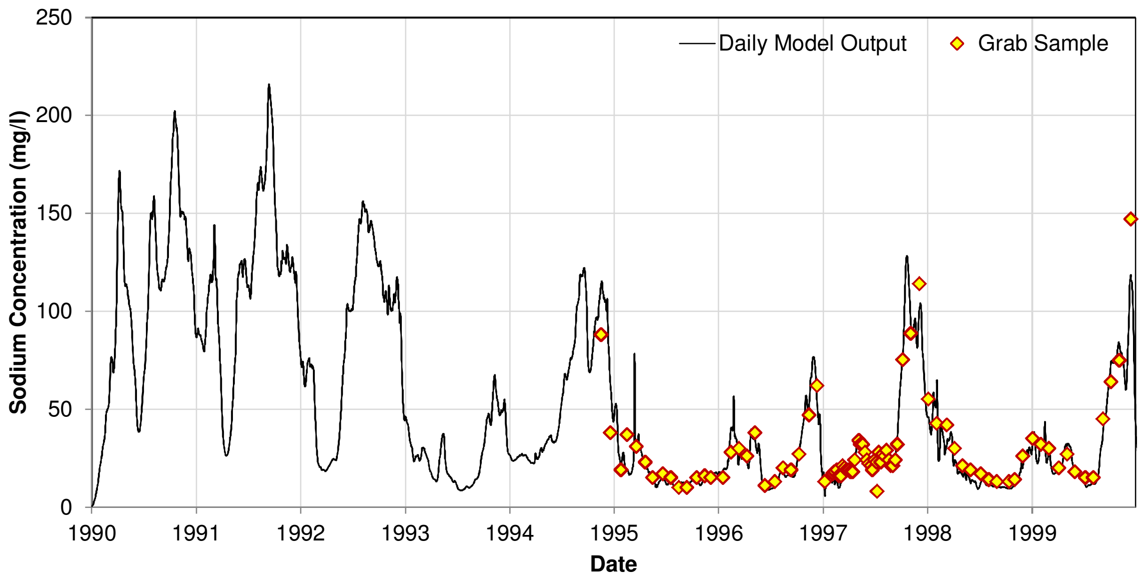

Figure 53a. Comparison Grab Sample Data and Simulated Daily Average Sodium Concentration in Old River at Bacon Island

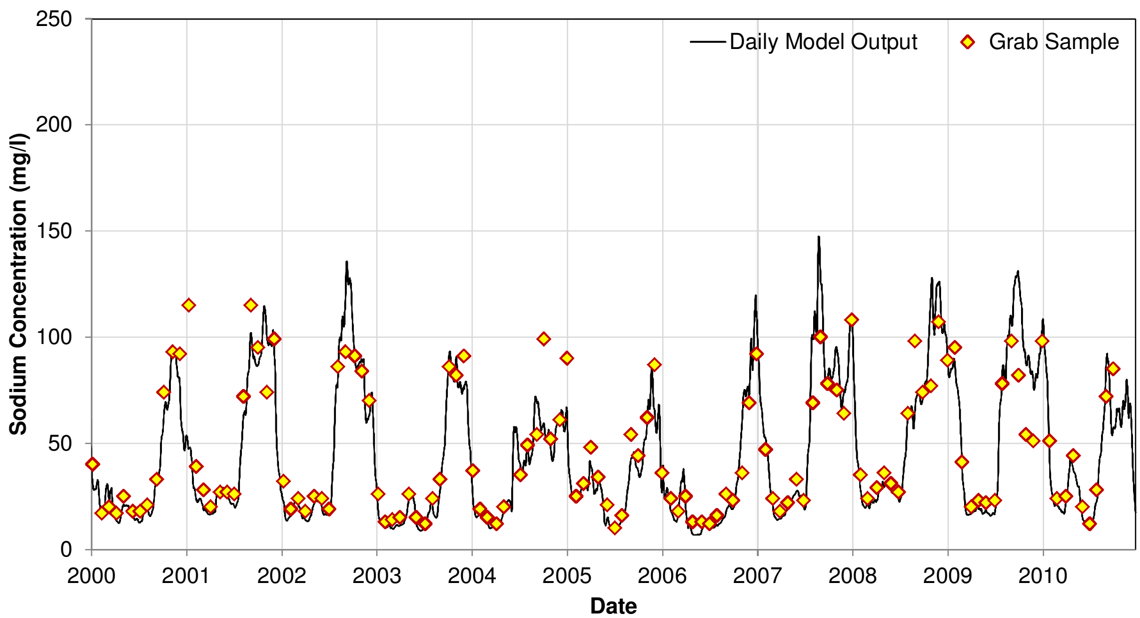

Figure 53b. Comparison Grab Sample Data and Simulated Daily Average Sodium Concentration in Old River at Bacon Island

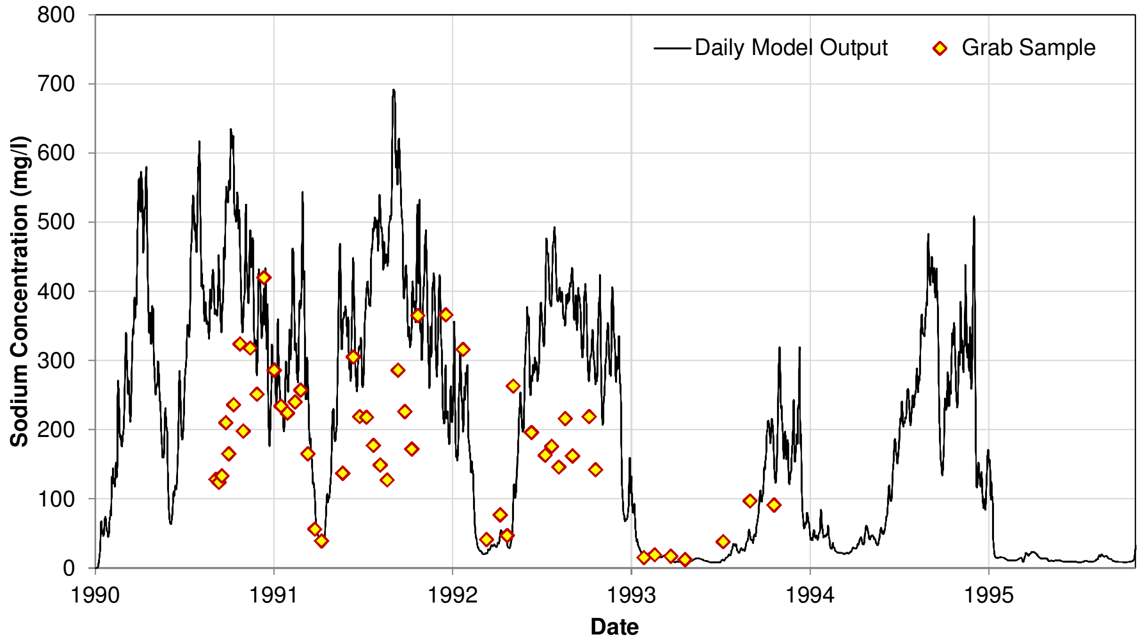

Figure 54. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration in San Joaquin River at Jersey Point

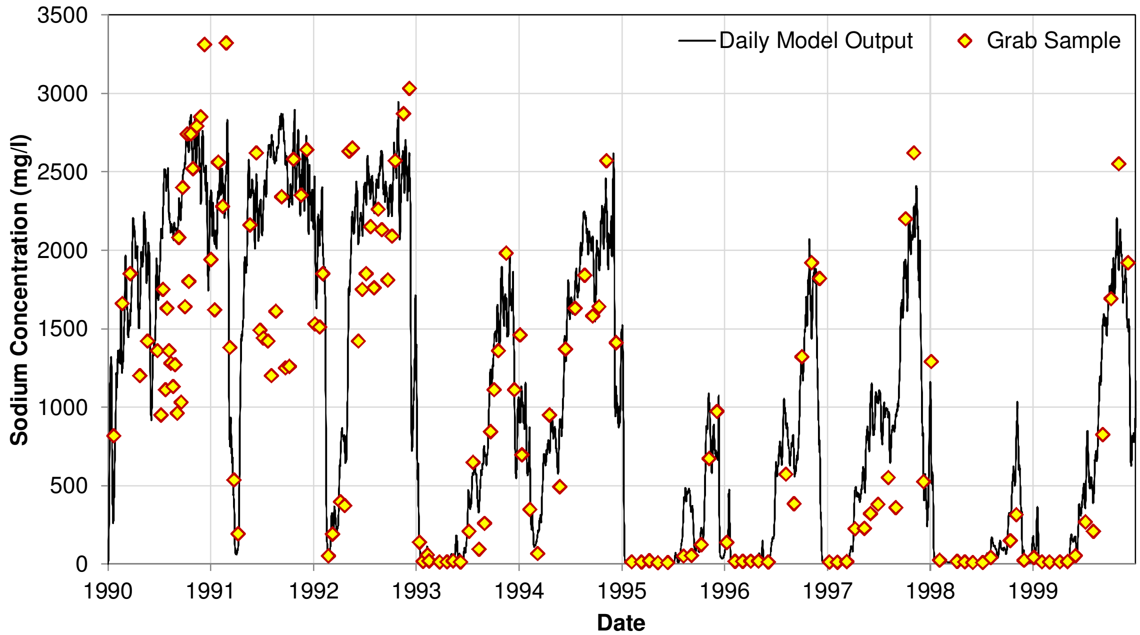

Figure 55a. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration in Sacramento River at Mallard Island

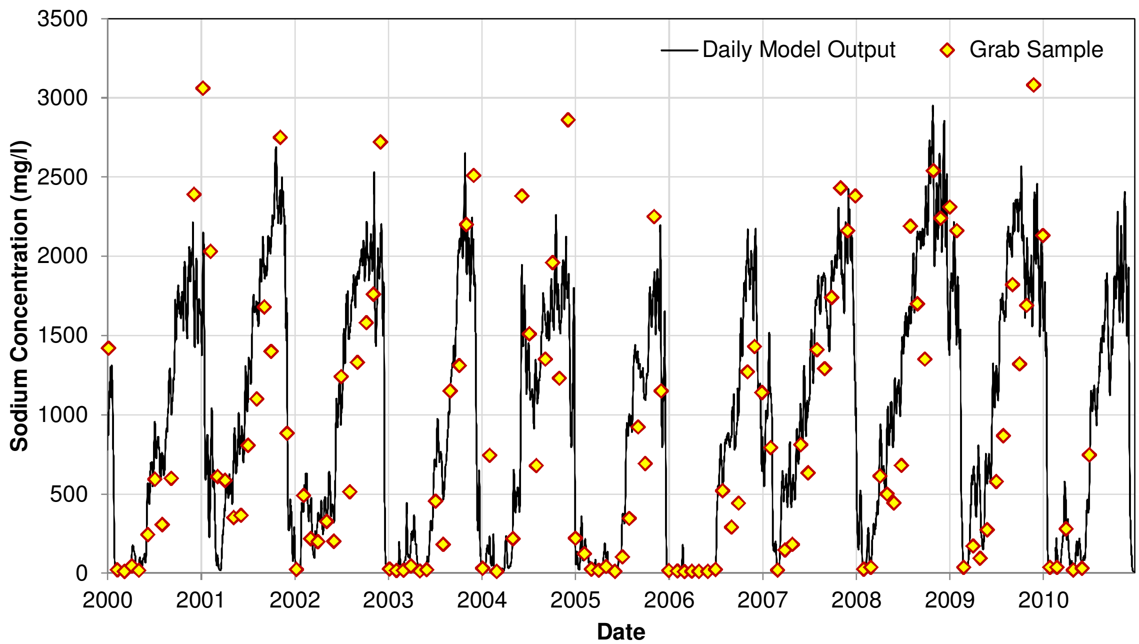

Figure 55b. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration in Sacramento River at Mallard Island

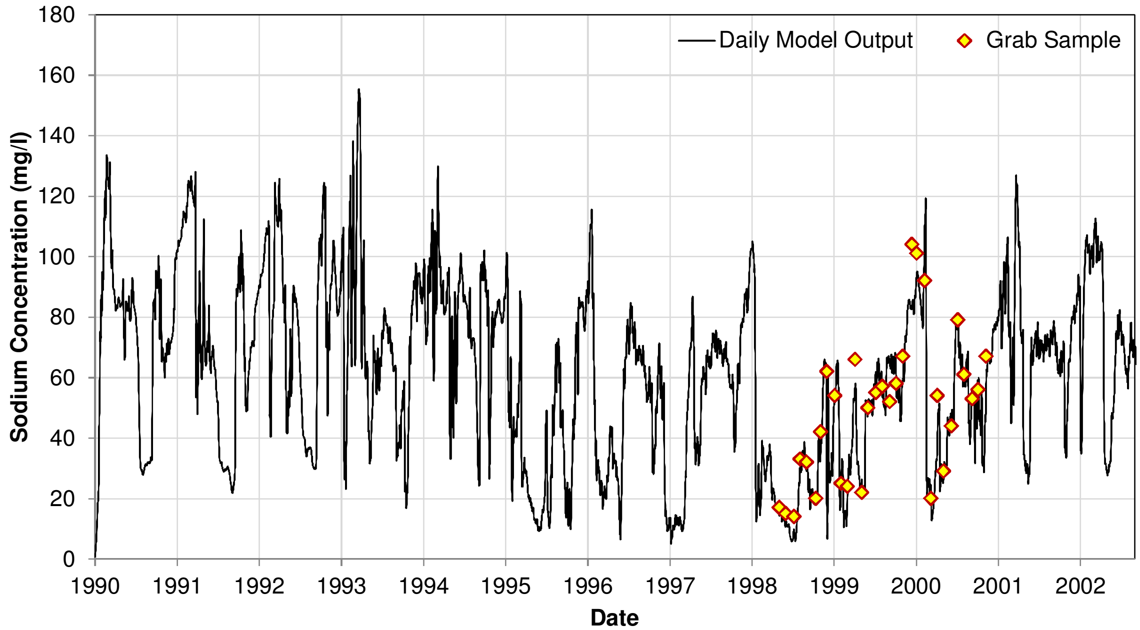

Figure 56. Comparison of Grab Sample Data and Simulated Daily Average Sodium Concentration in San Joaquin River at Highway 4

4.8 Alkalinity (As Bicarbonate)

This section provides a summary of model performances in simulating alkalinity concentrations at six Delta locations. Table 13 presents a summary of Bias, RMSE and NRMSE values for alkalinity simulations at the locations in the Delta. Based on average RMSE and NRMSE values, it is observed that the DSM2 model simulates alkalinity concentrations in the Delta reasonably well. As explained earlier in Section 4.1, the large NMRSE values in San Joaquin River may be related to deficiencies in the observed data. It is noted that there were only few grab sample data for alkalinity concentrations in San Joaquin River at Jersey Point compared to other locations. Average Bias values in Table 13 indicate that there is small trend of underestimation of observed alkalinity concentrations at the six locations in the Delta which can be also seen in the scatter plots presented in Figure 57. However, the model tends to underestimate at some locations and overestimate at other locations. Figures 58 through 63 show the time-series plots of grab sample data and simulated daily average alkalinity concentrations at the six Delta locations. From Figures 58 through 63, it can be seen that the model outputs follow the trend in observed data reasonably well. A review of the scatter plots and time-series plots indicate that the model is more accurate at simulating alkalinity concentration at lower salinity levels than at higher salinity levels.

Table 12. Validation Summary Statistics for Alkalinity Simulation at Different Locations in the Delta

Locations	Average Alkalinity as HCO3		Bias	RMSE	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L)	%	
Jones Pumping Plant	85.99	89.26	-3.27	21.63	19%	101
Banks Pumping Plant	84.27	85.21	-0.94	12.43	9%	152
Bacon Island	77.14	72.05	5.09	9.40	11%	274
San Joaquin River at Jersey Point	77.19	76.00	1.20	8.37	19%	11
Sacramento River at Mallard Island	84.19	79.80	4.39	9.32	14%	238
San Joaquin River at Highway 4	95.27	87.53	7.75	16.66	16%	32

Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

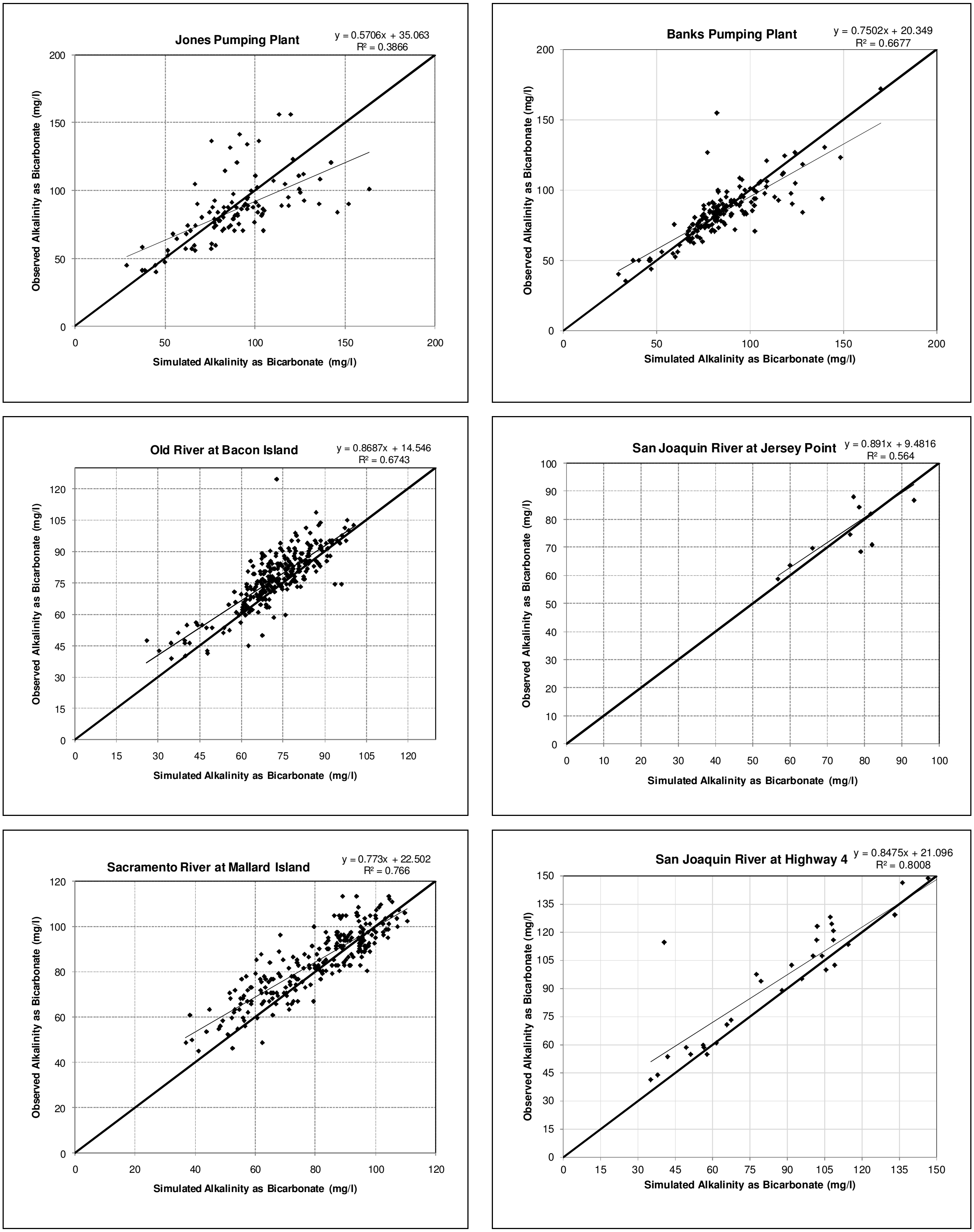

Figure 57. Scatter Plots Comparing Grab Samples and 15-Minute Model Outputs in the Delta

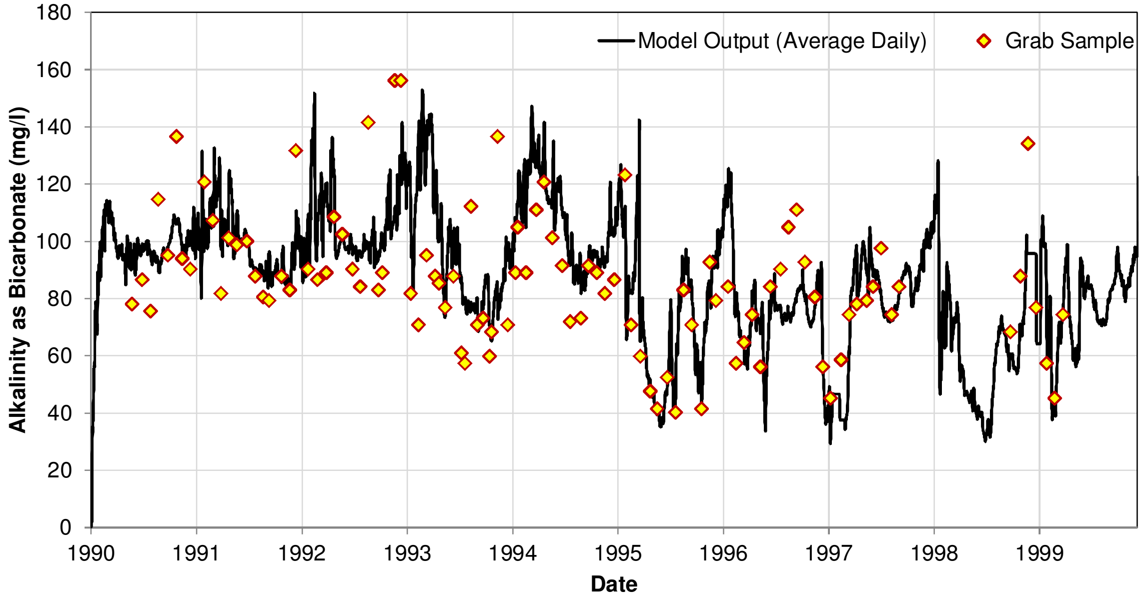

Figure 58. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity at Jones Pumping Plant

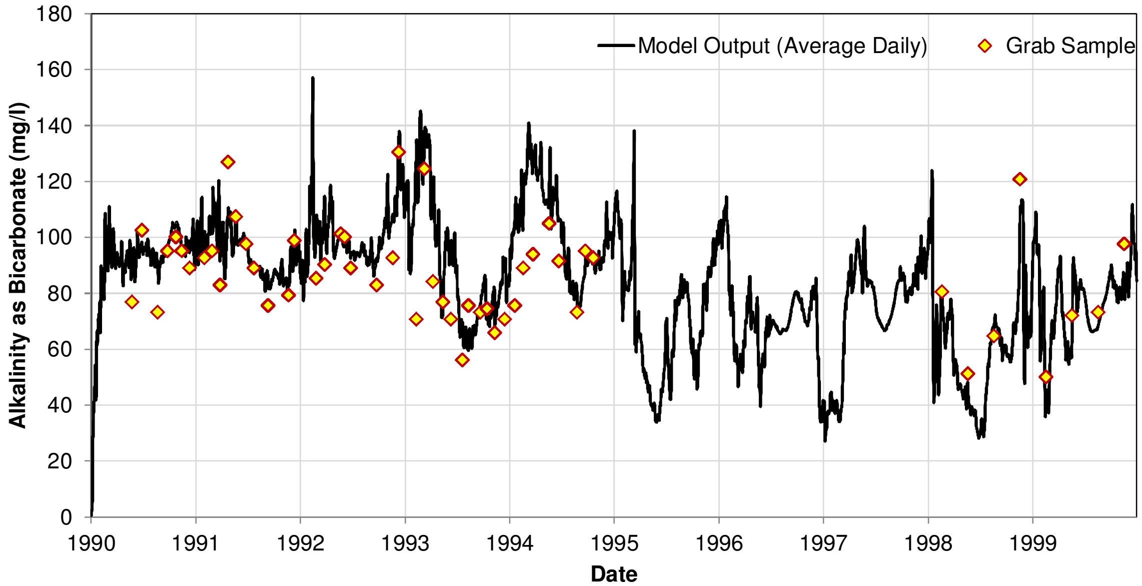

Figure 59a. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity at Banks Pumping Plant

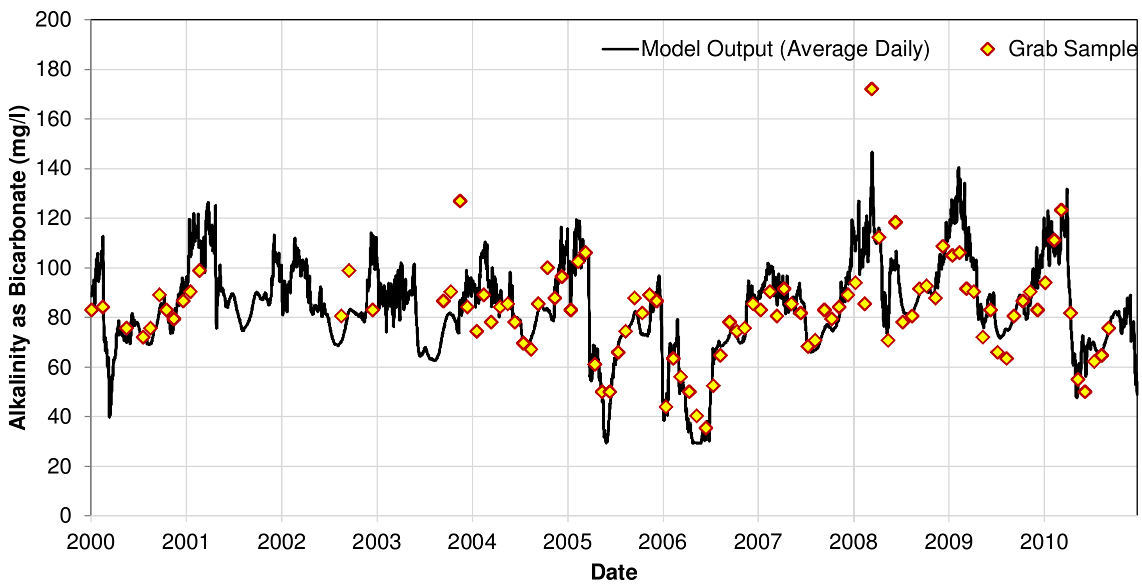

Figure 59b. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity at Banks Pumping Plant

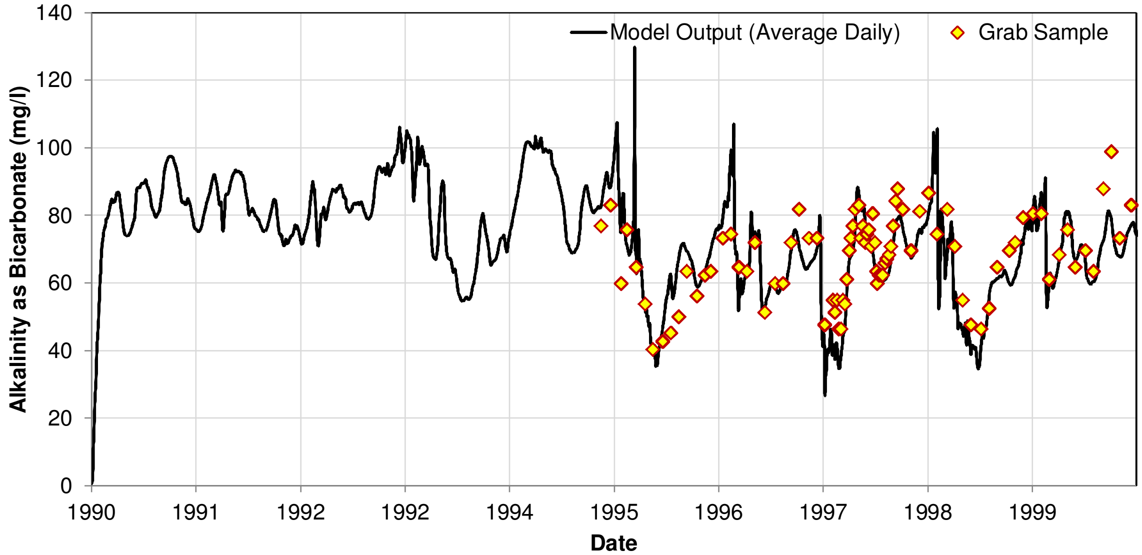

Figure 60a. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity in Old River at Bacon Island

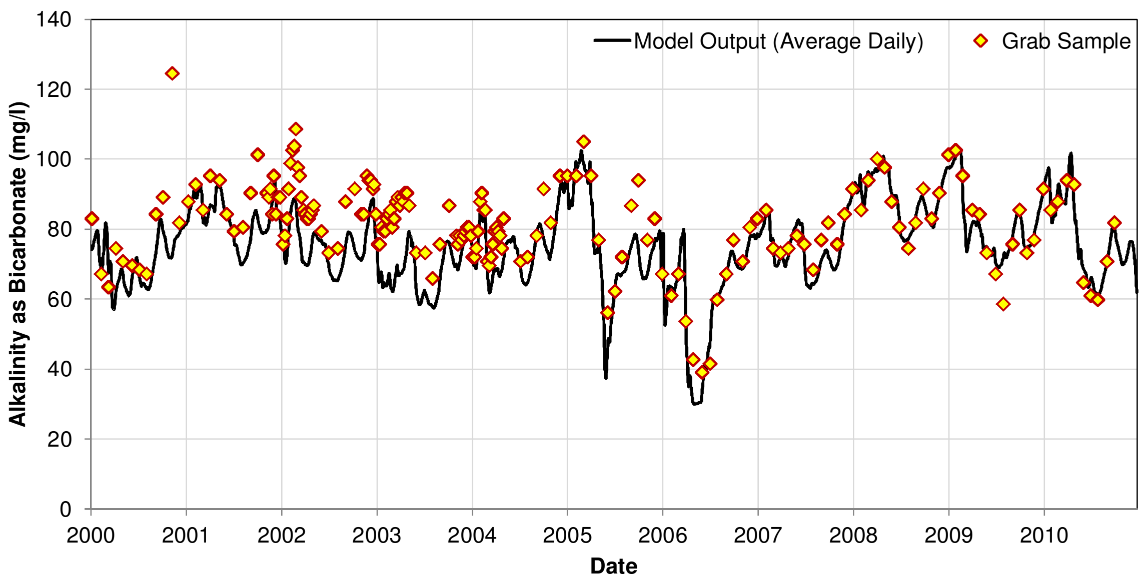

Figure 60b. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity in Old River at Bacon Island

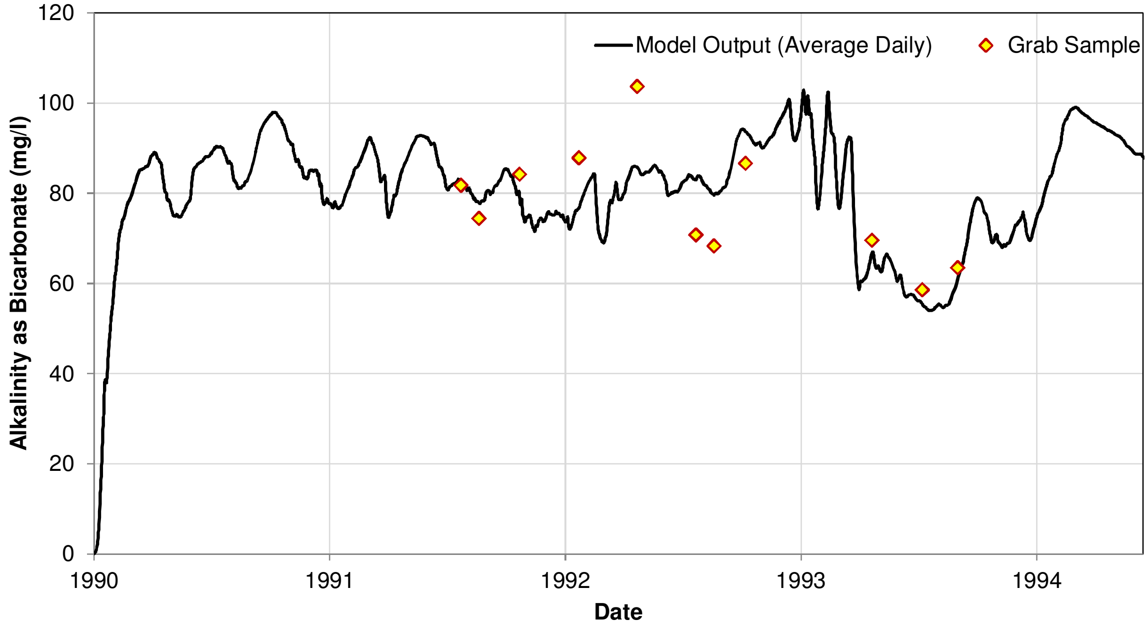

Figure 61. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity in San Joaquin River at Jersey Point

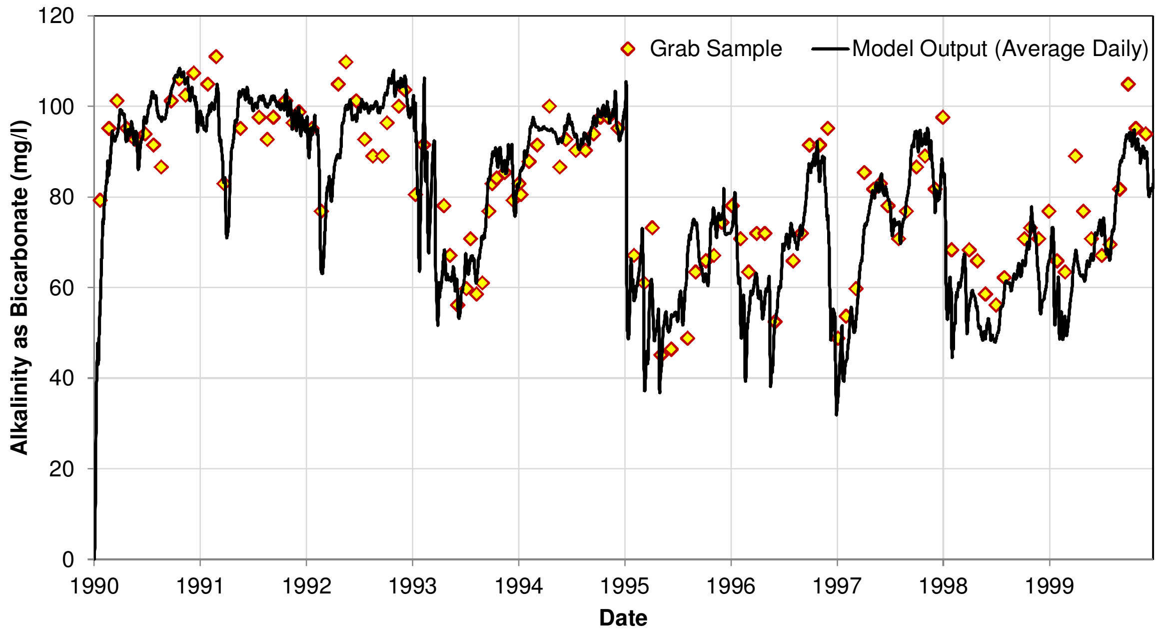

Figure 62a. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity in Sacramento River at Mallard Island

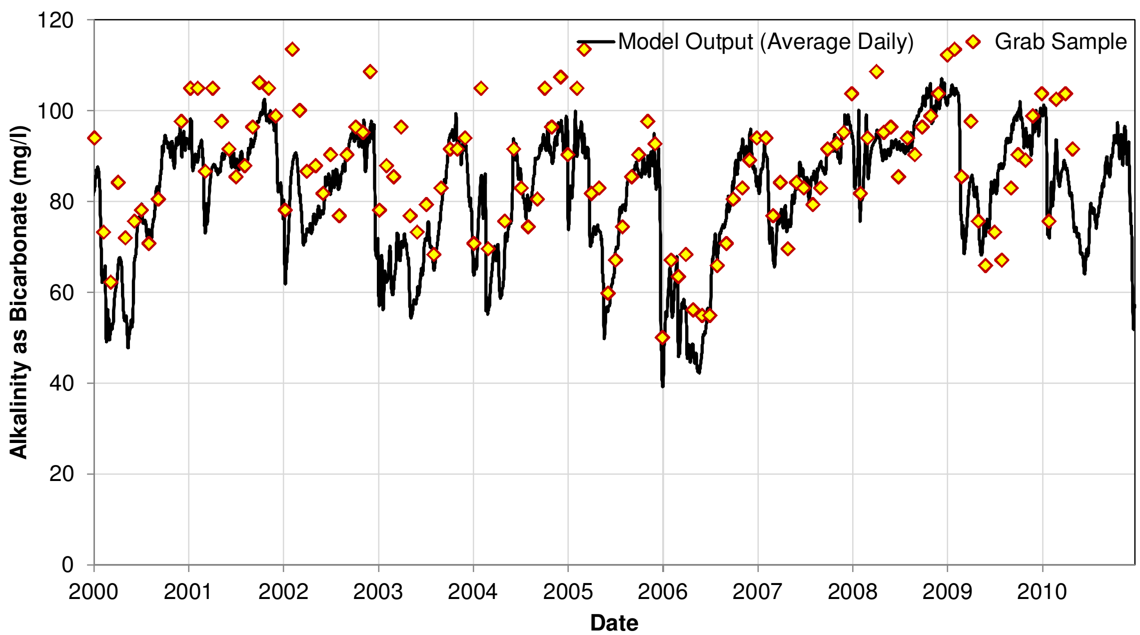

Figure 62b. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity in Sacramento River at Mallard Island

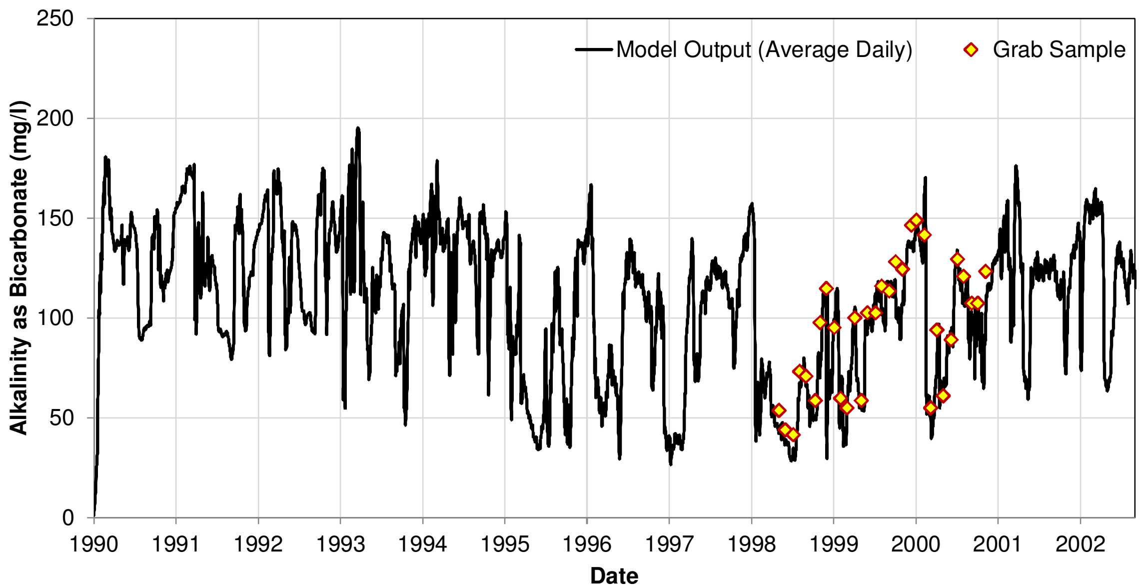

Figure 63. Comparison of Grab Sample Data and Simulated Daily Average Alkalinity in San Joaquin River at Highway 4

4.9 Simulation of EC vs. Cations and Anions

The cation and anion concentrations are simulated with a range of errors that is comparable to the errors associated with simulated EC values in DSM2. However, the model tends to overestimate cations and anions (except alkalinity) more frequently than EC at most of the Delta locations. Figure 59 shows a comparison of average NRMSE values for the eight water quality constituents based on results at the six Delta locations excluding San Joaquin River at Jersey Point. As seen in Figure 64, average NRMSE for anions (chloride, sulfate, bromide and alkalinity) is slightly higher than the average NRMSE for cations (calcium, magnesium and sodium) at the Delta locations. This variation in model performances may be caused by the propagation of observed inconsistencies (discussed in Section 2.3) in the water quality boundary data to the model outputs. However, statistical tests of significance may be required to verify if the errors associated with simulation of anions are significantly greater than the errors associated with simulation of cations. No statistical tests were performed due to lack of sufficient observed cation and anion data in the Delta. Overall, DSM2 is shown to be capable of simulating cations and anions with accuracy comparable to EC.

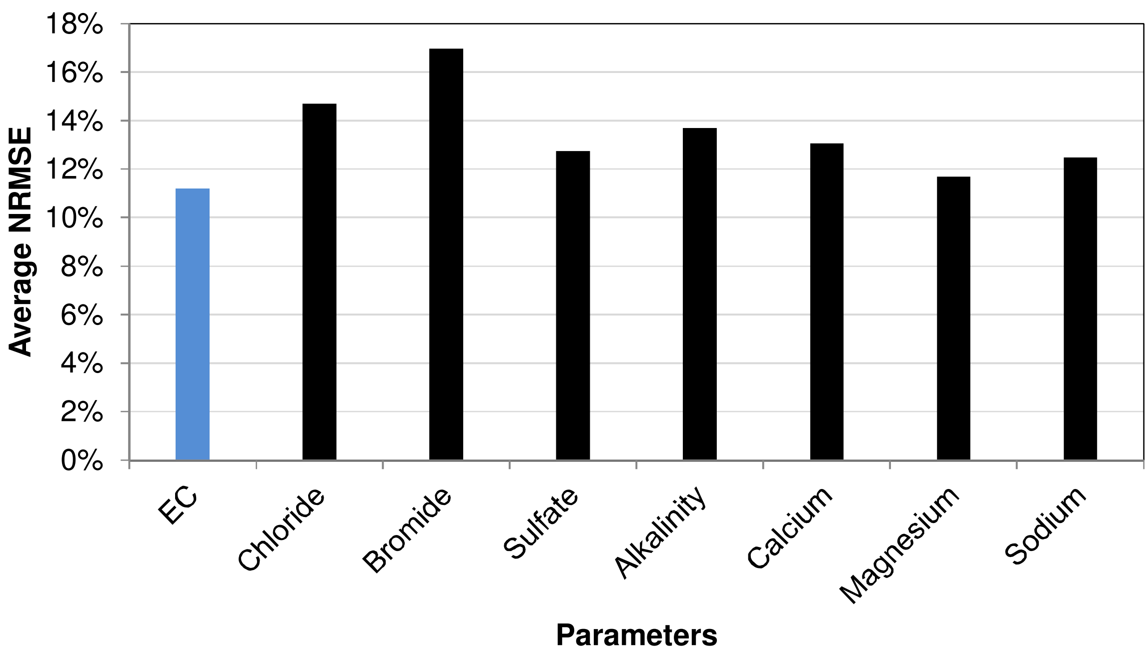

Figure 64. Comparison of EC Simulation Results Against Other Water Quality Constituents Using Average NRMSE Values

A review of the time-series plots (Sections 4.1 through 4.9) of simulated daily concentrations of cations and anions indicate that there are sudden increases in concentrations of ions, especially sulfate, bicarbonate, and calcium at certain Delta locations in the Old River at Bacon Island and at the Banks and Jones pumping plants. Figure 65 shows an example where there are spikes in simulated average daily sulfate concentrations in the Old River at Bacon

Island between 1995 and 1998. The spikes are observed to last not more than 2 days and they are noticed in time series plots of sulfate, calcium and alkalinity concentrations in the Old River at Bacon Island and at Banks and Jones pumping plants in the Delta.

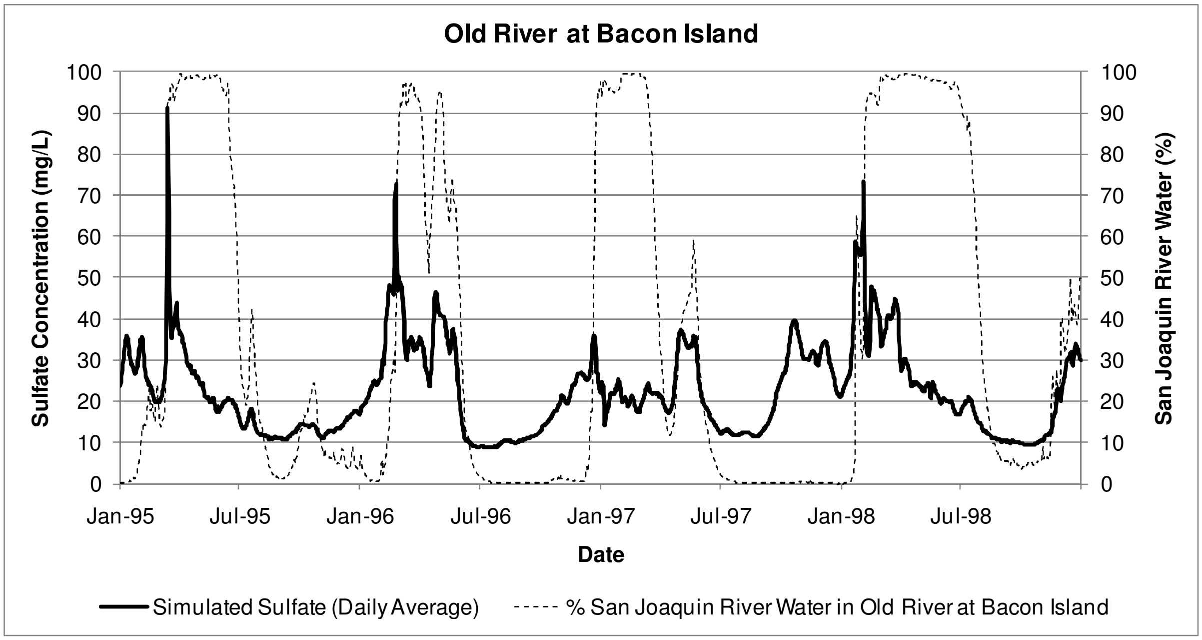

Figure 65. Graph showing Daily Simulated Sulfate Concentrations and San Joaquin River Water Proportion in the Old River at Bacon Island

Water quality in the Delta at any location is a result of complex mixing of different water sources. Therefore, a preliminary volumetric and constituent fingerprinting was performed to investigate the composition of water at a given location in the Delta. Figure QW shows the contribution of San Joaquin River water to total flow in the Old River at Bacon Island based on volumetric fingerprinting results. Fingerprinting results indicate that the observed spikes in the concentration of any water quality constituent in the Delta are associated with periods when there are sudden increases in the San Joaquin River flow at Vernalis combined with a relative surge in the respective constituent concentration in the San Joaquin River at Vernalis. Although there are similar changes in simulated concentrations of other cations and anions during these periods, the spikes are apparent only in sulfate, bicarbonate, and calcium daily plots. This observation can be explained by the fact that the proportion of sulfate, bicarbonate and calcium concentrations to the overall salinity is higher in the San Joaquin River at Vernalis when compared to sea water salinity distribution as shown in Figure 66.

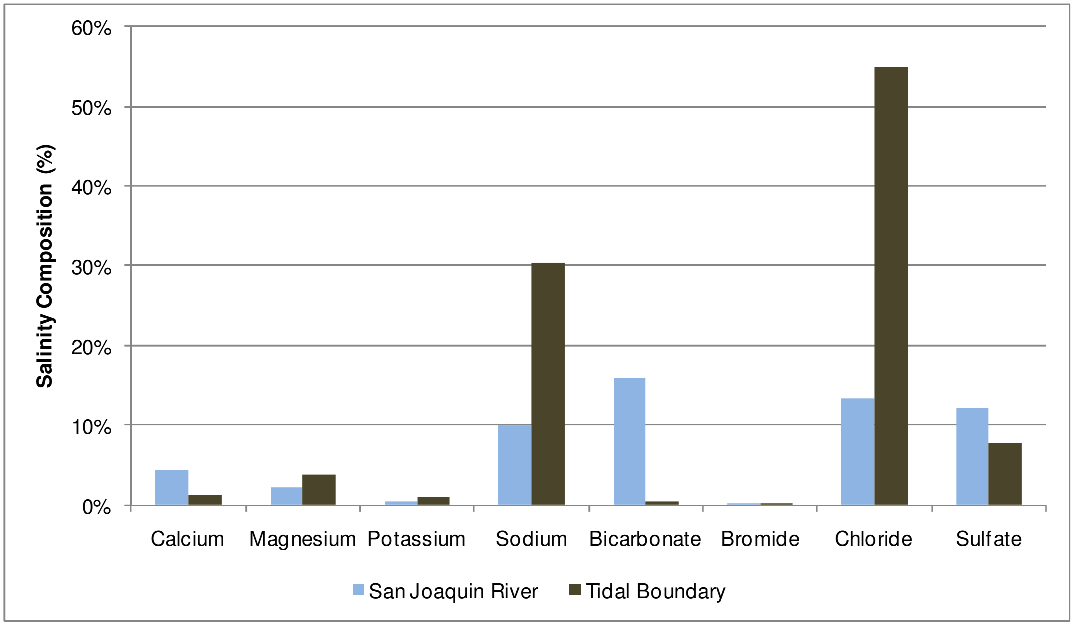

Figure 66. Salinity Constituents of Different Sources in the Delta

4.10 Seasonal Analysis

Table A1 in Attachment A summarizes average monthly NRMSE values at the locations in the Delta for the simulated water quality constituents. Results in Table A1 indicate that there tends to be a pattern of high NRMSE values in the summer months (June, July and August) for the water quality constituents including EC. Table A2 in Attachment A summarizes average monthly bias values at the locations in the Delta for the simulated water quality constituents including EC. Results in Table A2 indicate that there is a slight trend of overestimation of concentrations of cations and anions including EC in the summer periods. The results are inconclusive as there is no consistency either in the pattern of seasonal errors or overestimation in the summer. Monthly summary statistics reported in Tables A1 and A2 are based on limited observed data. Therefore, it is difficult to verify the model performances in simulating water quality under various seasonal flow and salinity conditions in the Delta.

4.11 Validation of DSM2's Simulation of Water Quality in the South Delta

Historically, the DSM2 model has been applied in many planning studies to investigate water quality in the South Delta especially at the Delta export locations where water quality is a primary concern for drinking water uses. This section presents a summary of the model performances in the Banks and Jones Pumping Plant locations. Average summary statistics for the water quality constituents are presented in Tables 13 and 14. A comparison of Tables 13 and 14 indicate that the average NRMSE values at the Jones Pumping Plant (21 percent) are greater than at the Banks Pumping Plant (12 percent). It is also observed that the water quality at Banks Pumping Plant is better than at Jones Pumping Plant based on average concentrations of cations and anions. No detailed investigations were performed to understand the reasons for the observed variation in model performances at these locations. Overall, average RMSE and NRMSE values for the two locations shown in Tables 13 and 14 indicate that the model results at the pumping locations are fairly accurate and match the observed data well.

Table 13. Summary Statistics for Jones Pumping Plant Based on Comparing Grab Sample Data and 15-Minute Model Outputs

Parameters	Average Concentration[1]		Bias[1]	RMSE[1]	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L))	%	
Electrical Conductivity	537	520	17	178	18%	140
Calcium	23.87	22.70	1.17	9.65	22%	135
Magnesium	14.87	14.77	0.10	4.55	17%	138
Sodium	59.88	62.90	-3.02	24.58	19%	135
Alkalinity (Bicarbonate)	85.99	89.26	-3.27	21.63	19%	101
Bromide	0.27	0.32	-0.05	0.13	23%	133
Chloride	81.75	95.84	-14.08	40.08	24%	142
Sulfate	48.35	44.75	3.60	29.28	25%	101

Note:
[1]Electrical conductivity in µS/cm
Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

Table 14. Summary Statistics for Banks Pumping Plant Based on Comparing Grab Sample Data and 15-min Model Outputs

Parameters	Average Concentration[1]		Bias[1]	RMSE[1]	NRMSE	Samples
	Observed (mg/L)	Simulated (mg/L)	(mg/L)	(mg/L))	%	
Electrical Conductivity	463	436	27	117	13%	162
Calcium	19.09	19.92	-0.83	4.34	11%	152
Magnesium	12.77	13.04	-0.27	2.52	10%	152
Sodium	50.01	49.85	0.16	16.20	14%	154
Alkalinity (Bicarbonate)	84.27	85.21	-0.94	12.43	9%	152
Bromide	0.22	0.25	-0.02	0.08	14%	130
Chloride	73.54	77.68	-4.14	26.54	15%	156
Sulfate	36.45	36.50	-0.04	16.72	12%	152

Note:
[1]Electrical conductivity in µS/cm
Key:
NRMSE = normalized root mean square error
mg/L = milligrams per liter
RMSE = root mean square error

Continuous data for EC, chloride, bromide, and sulfate are available at Banks Pumping Plant for the period from October, 2007 to present. These continuous data downloaded from CDEC website were used to validate the DSM2 model for simulating EC, chloride, bromide, and sulfate concentrations at the Banks Pumping Plant. Figures 67 through 70 compare simulated daily average concentrations and observed data at Banks Pumping Plant for the above-mentioned constituents. Results show that the model performs well in simulating EC and other ions at the Banks Pumping Plant. The observed bromide data shows few grab sample (less than 1 percent) with relatively high values that are not seen in the simulated bromide concentrations at the Banks Pumping Plant. Overall, this comparison using continuous data at Banks Pumping Plant supports the earlier conclusions that the model performs reasonably well in simulating cations and anions.

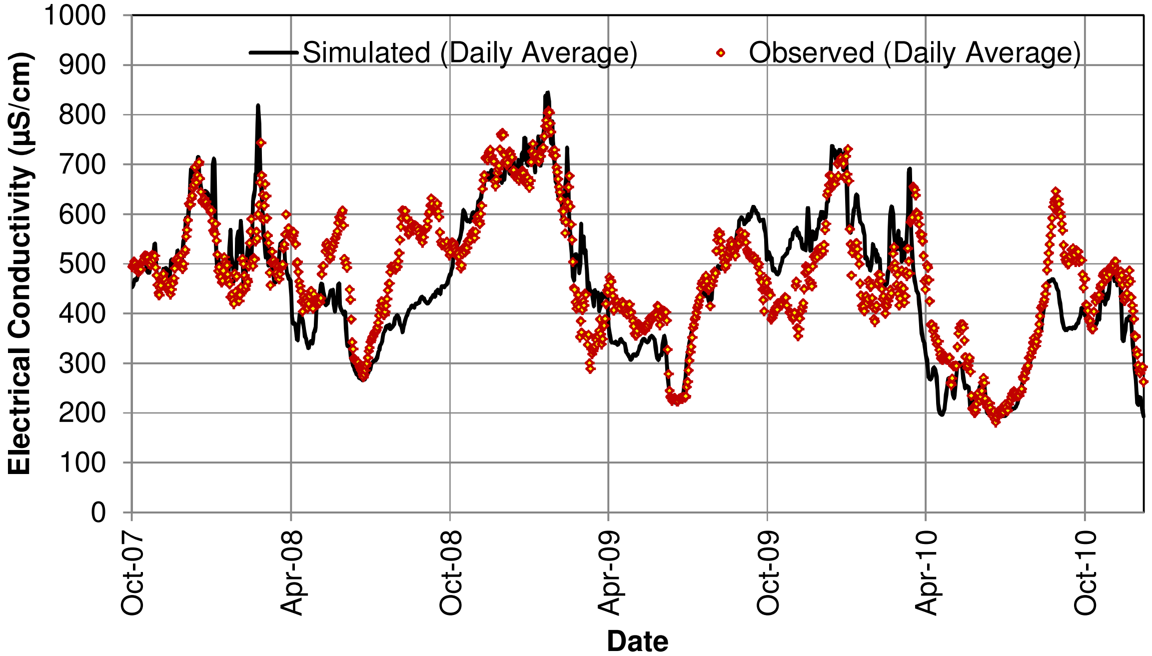

Figure 67. Comparison of Simulated and Observed Daily Electrical Conductivity Values at Banks Pumping Plant

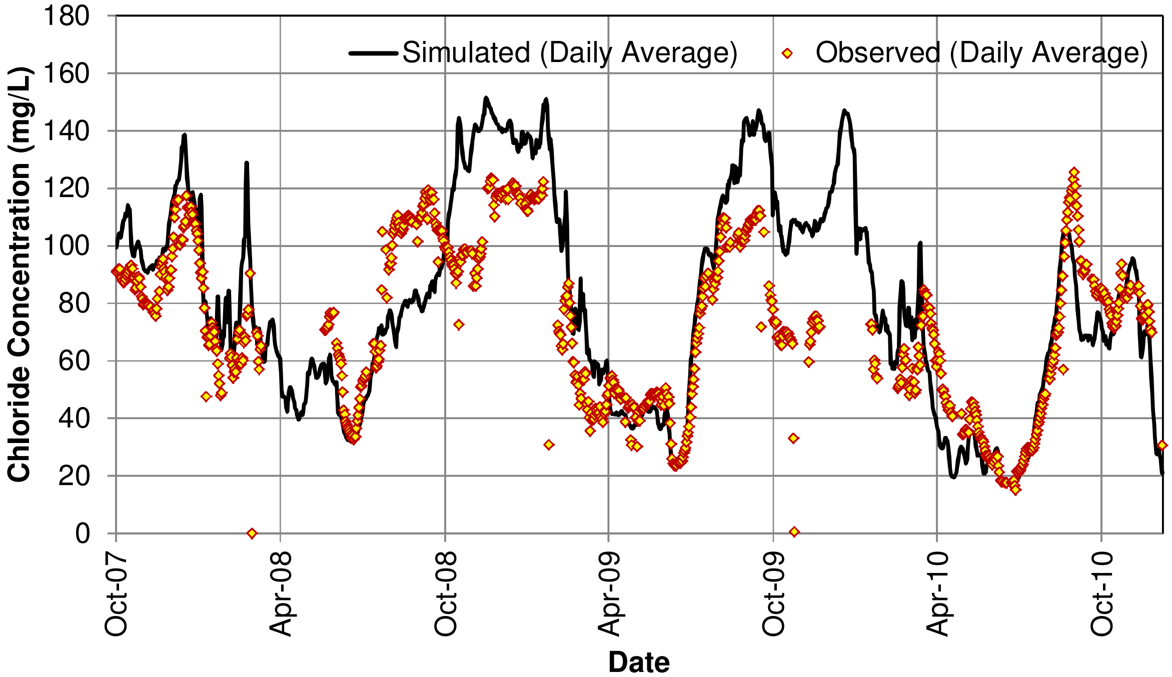

Figure 68. Comparison of Simulated and Observed Daily Chloride Concentration at Banks Pumping Plant

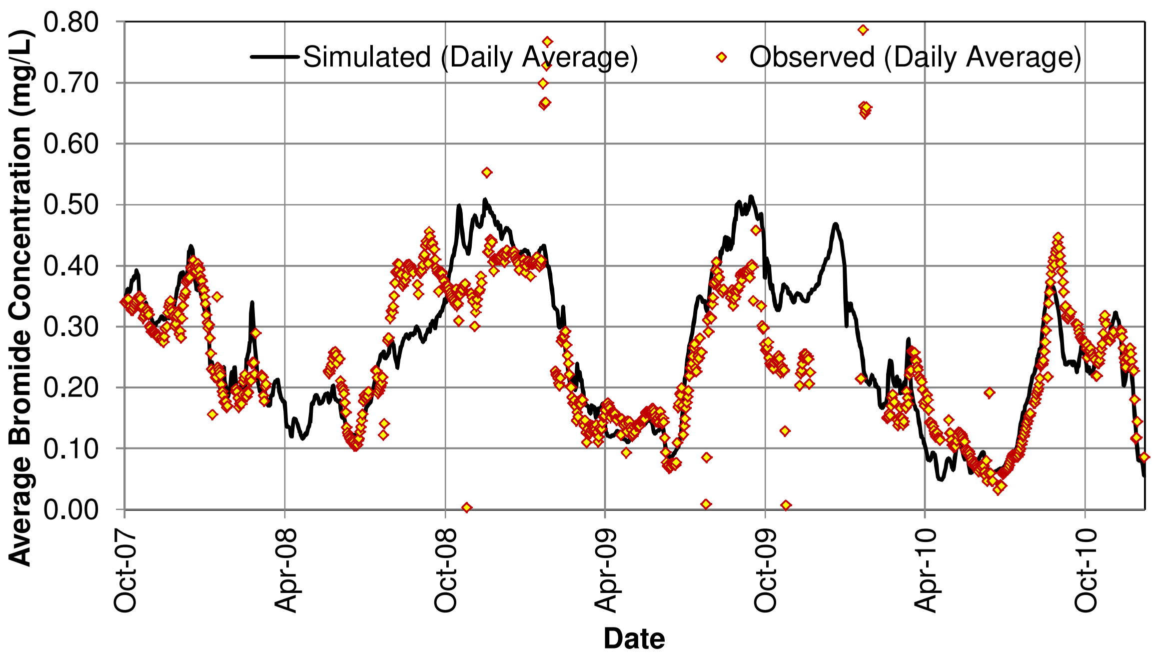

Figure 69. Comparison of Simulated and Observed Daily Bromide Concentration at Banks Pumping Plant

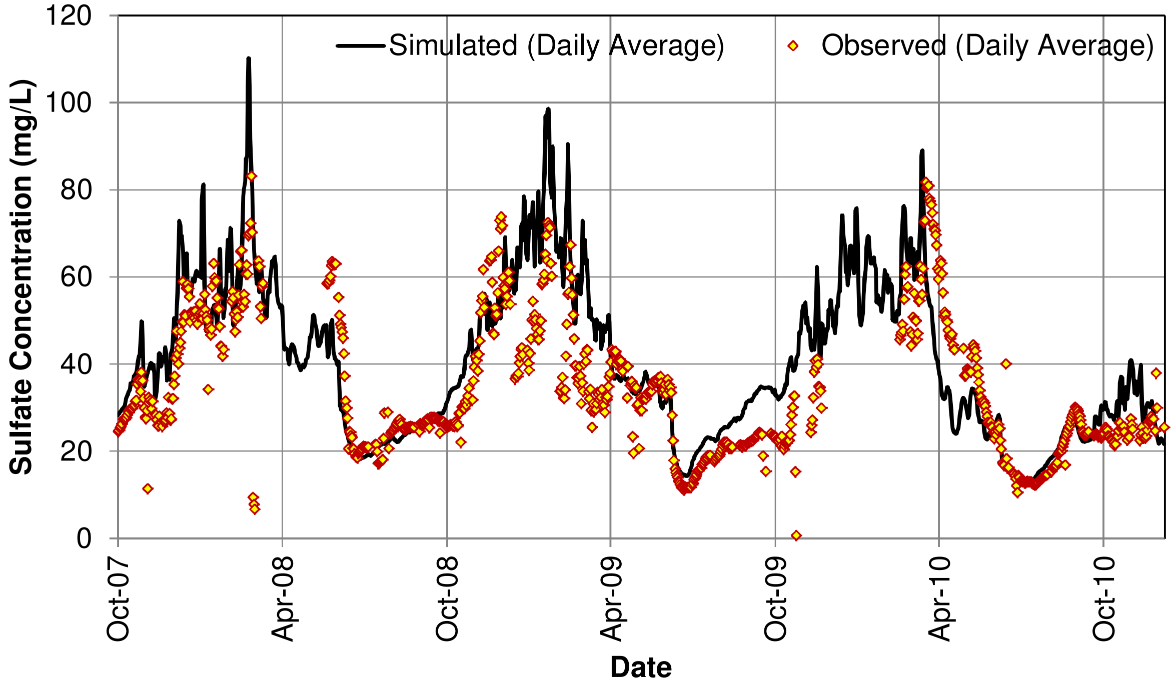

Figure 70. Comparison of Simulated and Observed Daily Sulfate Concentration at Banks Pumping Plant

5.0 Conclusions and Recommendations

This study evaluated the ability of the DSM2 model (Version 8.0.4) to simulate the transport of seven cations and anions based on input data that were collected and made available by DWR BDO at six different Delta locations. The validation effort is based on limited available monitoring data on cations and anions in the Delta, which do not adequately cover the range of seasonal flow and salinity conditions.

Historical validation efforts have demonstrated that the DSM2 model is capable of simulating EC reasonably well, which is also confirmed by this study. The results of this study also showed that the DSM2 model performs equally well in simulating cation and anion concentrations in the Delta. The range and magnitude of errors in the simulation of cations and anions are comparable to EC simulation results at the six Delta locations. However, DSM2 tends to overestimate the anion and cation concentrations, except alkalinity in the Delta more frequently than EC. The DSM2 model seems to produce better results for the cations and anions at lower salinity than at higher salinity conditions in the Delta. In the south Delta locations, DSM2 tends to underestimate EC, based on average NRMSE values.

The recommendations of this study are:

- Collect more observed cation and anion data for validation in the Delta, especially in the San Joaquin River.
- Verify error statistics using tests of statistical significance to exclude the chance of randomness in the results, when sufficient data is available.
- Verify the differences in model performances at the Jones and Banks pumping plants using DSM2 volumetric and constituent fingerprinting methodology.

6.0 References

California Department of Water Resources (DWR), 1995. Representative Delta Island Return Flow Quality for Use in DSM2, Memorandum Report.

Hem, J.D. 1985 Study and Interpretation of the Chemical Characteristics of Natural Water, USGS Water-Supply Paper 2254, Third Edition, U.S Government Printing Office.

Nader-Tehrani, P. 2001. "Chapter 2: DSM2 Calibration and Validation." Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh. 22nd Annual Progress Report to the State Water Resources Control Board. California Department of Water Resources, Office of State Water Project Planning, Sacramento, CA

Suits, B 2002. Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh, 23rd Annual Progress Report, Chapter 6: Calibrating DSM2-QUAL Dispersion Factors to Practical Salinity. June

Thein, M and Parviz Nader-Tehrani 2006. Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh, 27th Annual Progress Report, Chapter 9:DSM2 Simulation of Historical Delta Conditions over the 1975 – 1990 Period. October

.

Attachment A
Monthly Model Error Summary

Table A1. Monthly Average NRMSE Values at Different Locations in the Delta

Location	Parameter	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Old River at Bacon Island	Alkalinity	10%	13%	13%	9%	10%	16%	9%	7%	8%	5%	11%	19%
Old River at Bacon Island	Bromide	3%	2%	2%	1%	2%	7%	3%	5%	2%	1%	1%	7%
Old River at Bacon Island	Sulfate	11%	12%	6%	4%	8%	9%	9%	7%	8%	2%	8%	9%
Old River at Bacon Island	Magnesium	18%	7%	4%	4%	12%	13%	15%	6%	6%	3%	13%	13%
Old River at Bacon Island	Chloride	14%	3%	2%	2%	9%	9%	15%	16%	16%	4%	10%	7%
Old River at Bacon Island	Sodium	14%	3%	3%	2%	12%	13%	13%	4%	3%	2%	13%	13%
Old River at Bacon Island	Electrical Conductivity	13%	6%	5%	3%	13%	10%	14%	9%	11%	8%	9%	9%
Old River at Bacon Island	Calcium	11%	16%	9%	9%	11%	6%	8%	13%	14%	8%	11%	6%
Old River at Bacon Island	Average	12%	8%	6%	4%	10%	10%	11%	8%	9%	4%	10%	10%
Banks Pumping Plant	Alkalinity	16%	10%	6%	4%	15%	9%	6%	18%	7%	4%	7%	7%
Banks Pumping Plant	Bromide	15%	11%	4%	15%	14%	15%	7%	12%	5%	12%	14%	14%
Banks Pumping Plant	Calcium	17%	12%	8%	4%	16%	9%	7%	20%	7%	2%	8%	7%
Banks Pumping Plant	Chloride	17%	13%	5%	18%	16%	12%	14%	13%	4%	9%	12%	16%
Banks Pumping Plant	Electrical Conductivity	20%	12%	7%	8%	12%	8%	11%	18%	5%	11%	12%	11%
Banks Pumping Plant	Magnesium	13%	8%	6%	10%	12%	10%	8%	13%	4%	5%	9%	7%
Banks Pumping Plant	Sodium	19%	14%	6%	13%	18%	11%	12%	20%	4%	8%	12%	8%
Banks Pumping Plant	Sulfate	19%	14%	7%	11%	18%	10%	5%	22%	5%	2%	4%	4%
Banks Pumping Plant	Average	17%	12%	6%	10%	15%	10%	9%	17%	5%	6%	10%	9%
Jones Pumping Plant	Alkalinity	28%	15%	14%	11%	9%	18%	33%	16%	12%	12%	9%	19%
Jones Pumping Plant	Bromide	18%	15%	19%	13%	24%	37%	29%	25%	19%	16%	11%	23%
Jones Pumping Plant	Calcium	29%	24%	26%	22%	12%	23%	33%	21%	22%	24%	28%	12%
Jones Pumping Plant	Chloride	22%	13%	30%	12%	24%	39%	32%	26%	18%	15%	29%	13%
Jones Pumping Plant	Electrical Conductivity	22%	19%	23%	16%	15%	21%	24%	15%	15%	21%	25%	10%
Jones Pumping Plant	Magnesium	24%	17%	17%	14%	15%	21%	22%	15%	15%	16%	18%	8%

Table A1. Monthly Average NRMSE Values for Model Results at Different Locations in the Delta (contd.)

Location	Parameter	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Jones Pumping Plant	Sodium	20%	17%	23%	14%	17%	28%	24%	18%	18%	19%	23%	11%
Jones Pumping Plant	Sulfate	39%	37%	14%	15%	12%	23%	42%	19%	19%	15%	11%	25%
Jones Pumping Plant	Average	25%	20%	21%	14%	16%	26%	30%	19%	17%	17%	19%	15%
Sacramento River at Mallard Island	Alkalinity	15%	20%	15%	10%	7%	9%	15%	20%	14%	9%	8%	9%
Sacramento River at Mallard Island	Bromide	12%	5%	3%	5%	8%	10%	10%	18%	4%	6%	6%	9%
Sacramento River at Mallard Island	Calcium	4%	2%	2%	3%	6%	6%	6%	3%	3%	11%	5%	5%
Sacramento River at Mallard Island	Chloride	9%	3%	4%	6%	12%	19%	13%	6%	6%	4%	8%	19%
Sacramento River at Mallard Island	Electrical Conductivity	8%	4%	5%	6%	10%	11%	11%	5%	5%	4%	8%	9%
Sacramento River at Mallard Island	Magnesium	7%	3%	4%	6%	10%	11%	10%	6%	5%	6%	8%	9%
Sacramento River at Mallard Island	Sodium	8%	3%	5%	6%	10%	11%	11%	6%	5%	6%	7%	10%
Sacramento River at Mallard Island	Sulfate	9%	2%	6%	7%	7%	19%	13%	1%	7%	6%	7%	20%
Sacramento River at Mallard Island	Average	9%	5%	5%	6%	9%	12%	11%	8%	6%	6%	7%	11%
San Joaquin River at Highway 4	Alkalinity	2%	3%	1%	5%	5%	14%	2%	3%	1%	5%	5%	11%
San Joaquin River at Highway 4	Bromide	37%	14%	6%	35%	11%	47%	37%	16%	7%	43%	9%	55%
San Joaquin River at Highway 4	Calcium	10%	12%	4%	5%	8%	12%	10%	12%	3%	6%	7%	12%
San Joaquin River at Highway 4	Chloride	4%	18%	6%	9%	12%	7%	4%	18%	6%	10%	15%	9%
San Joaquin River at Highway 4	Electrical Conductivity	7%	14%	8%	7%	4%	7%	8%	15%	3%	11%	4%	2%
San Joaquin River at Highway 4	Magnesium	7%	13%	4%	3%	8%	9%	7%	13%	4%	3%	7%	9%
San Joaquin River at Highway 4	Sodium	6%	5%	2%	3%	8%	9%	6%	5%	2%	3%	10%	11%
San Joaquin River at Highway 4	Sulfate	4%	11%	7%	3%	6%	6%	4%	8%	8%	4%	7%	25%
San Joaquin River at Highway 4	Average	10%	11%	5%	9%	8%	14%	10%	11%	4%	11%	8%	17%

Table A1. Monthly Average NRMSE Values at Different Locations in the Delta (contd.)

Location	Parameter	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
San Joaquin River at Jersey Point	Alkalinity	24%	N/A	N/A	14%	N/A	N/A	23%	8%	N/A	N/A	N/A	N/A
San Joaquin River at Jersey Point	Bromide	12%	8%	18%	15%	45%	59%	31%	6%	12%	17%	12%	31%
San Joaquin River at Jersey Point	Calcium	9%	3%	9%	8%	19%	29%	15%	20%	30%	8%	11%	11%
San Joaquin River at Jersey Point	Chloride	13%	9%	19%	16%	46%	70%	33%	2%	10%	18%	26%	26%
San Joaquin River at Jersey Point	Electrical Conductivity	18%	2%	16%	12%	32%	50%	23%	34%	17%	13%	20%	14%
San Joaquin River at Jersey Point	Magnesium	8%	4%	13%	11%	28%	42%	19%	31%	26%	11%	15%	14%
San Joaquin River at Jersey Point	Sodium	13%	5%	18%	15%	42%	63%	29%	3%	10%	16%	25%	23%
San Joaquin River at Jersey Point	Sulfate	11%	N/A	N/A	N/A	4%	N/A	73%	4%	N/A	N/A	N/A	N/A
San Joaquin River at Jersey Point	Average	13%	5%	15%	13%	31%	52%	31%	13%	18%	14%	18%	20%

Key:
N/A –Data not available
Highlighted cells indicate the maximum NRMSE value for a given parameter at a given location

Table A2. Monthly Average Bias at different locations in the Delta

Location	Parameter	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Bacon Island	Alkalinity (mg/L)	4	8	9	3	5	7	5	3	5	1	7	12
Bacon Island	Bromide (mg/L)	0	0	0	0	0	0	0	0	0	0	0	0
Bacon Island	Calcium (mg/L)	0	1	-1	-1	0	0	0	1	0	-1	0	0
Bacon Island	Chloride (mg/L)	10	3	2	2	2	-10	12	-17	-21	-2	4	-5
Bacon Island	Electrical Conductivity	74	37	35	23	61	-1	61	52	68	47	59	25
Bacon Island	Magnesium (mg/L)	1	1	0	0	0	-2	1	0	0	0	-1	-2
Bacon Island	Sodium (mg/L)	8	4	3	2	3	-11	7	3	4	3	3	-12
Bacon Island	Sulfate (mg/L)	3	4	2	1	0	-4	2	3	2	0	-1	-4
Bacon Island	Average	13	7	6	4	9	-3	11	6	7	6	9	2
Banks Pumping Plant	Alkalinity (mg/L)	2	-4	0	-4	4	0	-5	2	-2	-1	0	0
Banks Pumping Plant	Bromide (mg/L)	0	0	0	0	0	0	0	0	0	0	0	0
Banks Pumping Plant	Calcium (mg/L)	0	-2	1	-1	0	-1	-2	0	-1	0	-1	-1
Banks Pumping Plant	Chloride (mg/L)	10	-10	6	-14	-6	-11	5	-11	3	-4	-2	-2
Banks Pumping Plant	Electrical Conductivity	94	-9	55	-27	46	6	57	-33	30	30	4	47
Banks Pumping Plant	Magnesium (mg/L)	0	0	1	-1	0	-2	0	0	0	0	-1	-1
Banks Pumping Plant	Sodium (mg/L)	10	-2	6	-6	3	-4	6	0	3	-1	1	-3
Banks Pumping Plant	Sulfate (mg/L)	8	-1	6	5	3	3	1	2	2	0	-1	-2
Banks Pumping Plant	Average	16	-4	9	-6	7	-1	8	-5	4	3	0	5
Jones Pumping Plant	Alkalinity (mg/L)	-14	-10	-12	-2	-3	2	-3	-11	-11	-3	-4	4
Jones Pumping Plant	Bromide (mg/L)	0	0	0	0	0	0	0	0	0	0	0	0
Jones Pumping Plant	Calcium (mg/L)	-4	2	-4	4	1	1	2	3	0	3	-1	-2
Jones Pumping Plant	Chloride (mg/L)	-12	-1	-25	5	-13	-46	-30	-24	-8	9	-14	-12
Jones Pumping Plant	Electrical Conductivity	-32	72	-71	87	22	-71	-21	-13	36	116	-11	-20
Jones Pumping Plant	Magnesium (mg/L)	0	1	-1	2	0	-2	-1	0	0	2	0	-1

Table A2. Monthly Average Bias for model results at different locations in the Delta (contd.)

Location	Parameter	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Jones Pumping Plant	Sodium (mg/L)	-5	8	-12	8	-2	-23	-10	-9	3	13	-4	-7
Jones Pumping Plant	Sulfate (mg/L)	-10	12	-4	6	2	0	-5	-6	2	11	-3	6
Jones Pumping Plant	Average	-10	11	-16	14	1	-17	-8	-7	3	19	-5	-4
Mallard Island	Alkalinity (mg/L)	7	11	7	1	0	-1	6	12	5	1	0	1
Mallard Island	Bromide (mg/L)	0	0	0	0	-1	-1	0	-1	0	0	-1	-1
Mallard Island	Calcium (mg/L)	2	2	-1	-3	-9	-7	-4	-2	-2	4	-4	-4
Mallard Island	Chloride (mg/L)	38	38	-96	-74	-422	-515	-165	-174	-150	-32	-265	-297
Mallard Island	Electrical Conductivity	113	212	-128	41	-905	-592	-379	-279	-176	175	-519	-130
Mallard Island	Magnesium (mg/L)	0	5	-7	-6	-30	-30	-19	-11	-7	2	-21	-20
Mallard Island	Sodium (mg/L)	43	28	-34	-11	-200	-115	-37	-65	-27	-5	-128	-19
Mallard Island	Sulfate (mg/L)	19	2	-15	-5	-28	-19	11	-3	-24	-6	-35	8
Mallard Island	Average	28	37	-34	-7	-199	-160	-73	-66	-48	17	-122	-58
San Joaquin River at Highway 4	Alkalinity (mg/L)	2	-4	0	-4	4	0	-5	2	-2	-1	0	0
San Joaquin River at Highway 4	Bromide (mg/L)	0	0	0	0	0	0	0	0	0	0	0	0
San Joaquin River at Highway 4	Calcium (mg/L)	0	-2	1	-1	0	-1	-2	0	-1	0	-1	-1
San Joaquin River at Highway 4	Chloride (mg/L)	10	-10	6	-14	-6	-11	5	-11	3	-4	-2	-2
San Joaquin River at Highway 4	Electrical Conductivity	40	-47	27	12	26	48	51	-50	-25	45	21	8
San Joaquin River at Highway 4	Magnesium (mg/L)	0	0	1	-1	0	-2	0	0	0	0	-1	-1
San Joaquin River at Highway 4	Sodium (mg/L)	10	-2	6	-6	3	-4	6	0	3	-1	1	-3
San Joaquin River at Highway 4	Sulfate (mg/L)	8	-1	6	5	3	3	1	2	2	0	-1	-2
San Joaquin River at Highway 4	Average	9	-8	6	-1	4	4	7	-7	-3	5	2	0

Table A2. Monthly Average Bias for model results at different locations in the Delta (contd.)

Location	Parameter	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
San Joaquin River at Jersey Point	Alkalinity (mg/L)	11	N/A	N/A	-7	N/A	N/A	-11	4	N/A	N/A	N/A	N/A
San Joaquin River at Jersey Point	Bromide (mg/L)	0	0	0	0	-1	-1	-1	0	0	0	0	-1
San Joaquin River at Jersey Point	Calcium (mg/L)	2	0	-1	-2	-7	-10	-4	-4	6	-1	-2	-4
San Joaquin River at Jersey Point	Chloride (mg/L)	75	-51	-71	-86	-320	-456	-176	11	37	-56	-143	-187
San Joaquin River at Jersey Point	Electrical Conductivity	407	11	-234	-147	-785	-1124	-342	-497	335	-45	-340	-360
San Joaquin River at Jersey Point	Magnesium (mg/L)	4	-2	-5	-7	-21	-28	-10	-15	9	-5	-8	-11
San Joaquin River at Jersey Point	Sodium (mg/L)	43	-17	-35	-41	-161	-229	-83	8	20	-32	-72	-95
San Joaquin River at Jersey Point	Sulfate (mg/L)	7	N/A	N/A	N/A	3	N/A	-54	3	N/A	N/A	N/A	N/A
San Joaquin River at Jersey Point	Average	69	-10	-58	-41	-185	-308	-85	-61	68	-23	-94	-110

Key:
N/A –Data not available