Methodology for Flow and Salinity Estimates in the Sacramento-San Joaquin Delta and Suisun Marsh

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Chapter 5
Estimating Delta-wide Bromide Using DSM2- Simulated EC Fingerprints

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Contents

Figures

Tables

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5 Estimating Delta-wide Bromide Using DSM2-Simulated EC Fingerprints

5.1 Introduction

This chapter compares 6 methods to determine bromide concentrations at select locations in the Sacramento-San Joaquin River Delta (the Delta). The results of the methods are compared to observed grab sample bromide data at those Delta locations. The 6 methods examined are shown in Table 5-1.

Table 5-1 Methods to Determine Bromide Concentrations

No.	Method	Description
1	DSM2 Simulation	Bromide is simulated at various Delta locations using DSM2 with bromide values as input at boundaries.
2	Direct EC-Br regression	Regression using EC and bromide observed data (does not consider source of EC in regression).
3	Previous BDO[a] regression	Linear regression using observed data (considered Volumetric fingerprint from Martinez).
4	Site-specific regression	DSM2 EC fingerprint simulations[b]. Results from multiple linear regressions developed from site data and from fingerprint results.
5	Regional regression	DSM2 EC Fingerprint simulations. Results from multiple linear regressions developed from regional data that include several sites and from DSM2 fingerprint output.
6	Delta-wide regression	DSM2 EC Fingerprint simulations. Results from multiple linear regressions developed using fingerprint output and with full Delta data.

[a] BDO Bay Delta Office
[b] Fingerprints provide the amount of electrical conductivity (EC) contributed by different sources of salinity, such as the ocean, agricultural returns, and river inflows. These sources contain different combinations of cations and anions. For example, the salinity coming from the ocean contains a higher proportion of bromide than that coming from river inflows.

5.2 Background

The dispersion coefficients in the current version of QUAL, the water quality module of DSM2, were calibrated using electrical conductivity, which measures the water's ability to conduct electrical current. At high salinity concentration, as usually occurs at DSM2's downstream boundary at Martinez, EC underestimates true salinity[1]. This has raised concerns about directly simulating truly conservative water quality constituents with DSM2's EC-based dispersion coefficients. Although no actual test has been conducted to evaluate this as a potential problem, some analysis has been done.

Recently, direct simulation of historical Delta bromide using DSM2 was conducted and reported by Montgomery Watson Harza (2011) as part of a larger analysis of DSM2's current capability to simulate various cations and anions. Cations and anions values were developed at model boundaries, including Martinez, by applying regressions developed by the California Department of Water Resources to DWR's historical EC simulation time series. Based on model results, MWH concluded that using DSM2 to simulate historical Delta cation and anion concentrations does not introduce additional error beyond the baseline error in EC.

As part of our review of MWH's report, we reproduced the direct simulation of bromide and compared values to observed bromide, but at more locations. In addition, we compared simulated bromide to bromide derived from multiple linear regressions based on simulated EC fingerprints and grab samples containing both EC and bromide. We considered 3 regressions: a single Delta-wide, site-specific, and regional.

As presented below, our analysis confirms MWH's conclusion that direct simulation of bromide with DSM2 and the current version of dispersion coefficients is equivalent to estimating bromide based on DSM2-simulated EC and applying multiple linear regressions based on simulated EC fingerprints. However, using observed EC and multiple linear regressions provides significantly better estimates of bromide. Multiple linear regressions based on Delta regions perform nearly as well as site-specific regressions and allow for converting from EC to bromide at nearly any location in the Delta.

[1] "An important drawback to using EC to calibrate dispersion factors is its acknowledged failure to behave as a truly conservative constituent of salinity. As salinity and ionic concentration increases, electrical conductance increases. For high concentrations, however, the proximity of ions to each other depresses their activity and consequently their ability to transmit electrical current. 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, Calibrating DSM2-QUAL Dispersion Factors to Practical Salinity (Chapter 6), 2002)

5.3 Directly Simulating Delta Bromide

We followed MWH's approach in setting up the DSM2 model to simulate bromide directly. Boundary conditions for bromide were generated using regression equations developed by the Bay-Delta Office (BDO) (work by Bob Suits, not published) based on grab sample bromide and EC data. The regressions for all boundaries are in the linear form

$$Br = A + B * EC \qquad \text{(Equation 1)}$$

where Br is the bromide concentration in mg/L; A and B are regression coefficients (y-axis intercept and slope, respectively); and EC is electrical conductivity in microsiemens per centimeter (µS/cm), or equally, micromhos per centimeter (µmhos/cm).

Figure 5-1 through Figure 5-3 show the scatterplots of EC and bromide and linear EC-bromide regressions represented by equation (1) at Martinez, Sacramento River at Freeport, and San Joaquin River at Vernalis. The regression for Sacramento River is also applied to Eastside Streams. The EC and bromide data used to derive the regression at Martinez were grab sample EC and bromide data at Mallard Island and Jersey Point downloaded from Water Data Library (WDL). The data used to develop the Sacramento River bromide-EC regression came from grab sample data at Delta Cross Channel, and Jersey Point and Mallard Island when EC < 300 uS/cm. The EC and bromide data used to derive the regression at San Joaquin River at Vernalis were grab sample data at San Joaquin River at Vernalis.

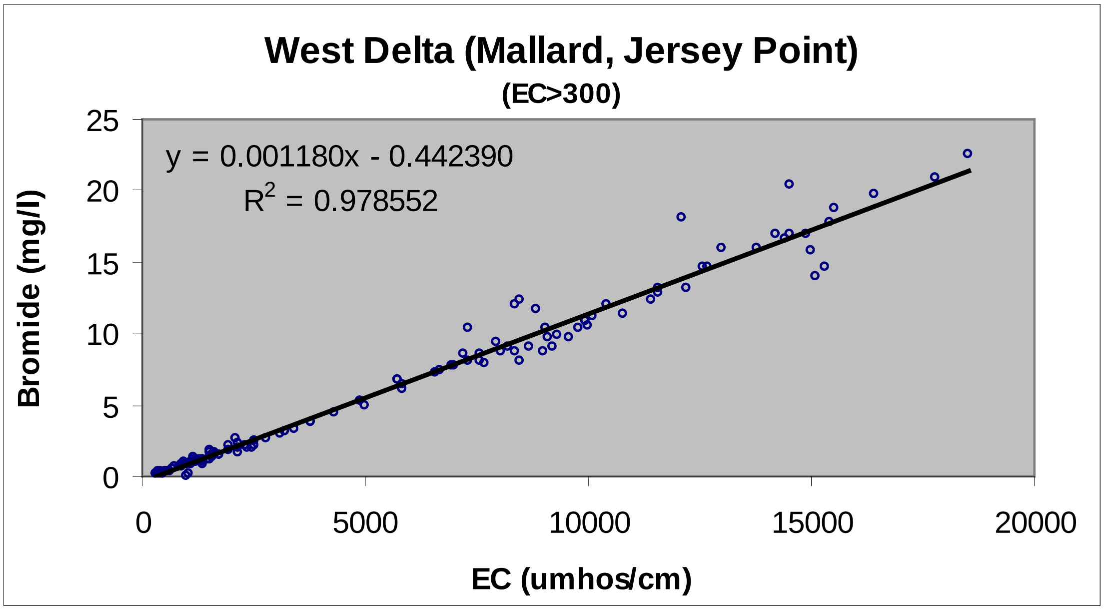


Figure 5-1 Martinez Regression Used for Converting from EC to Bromide

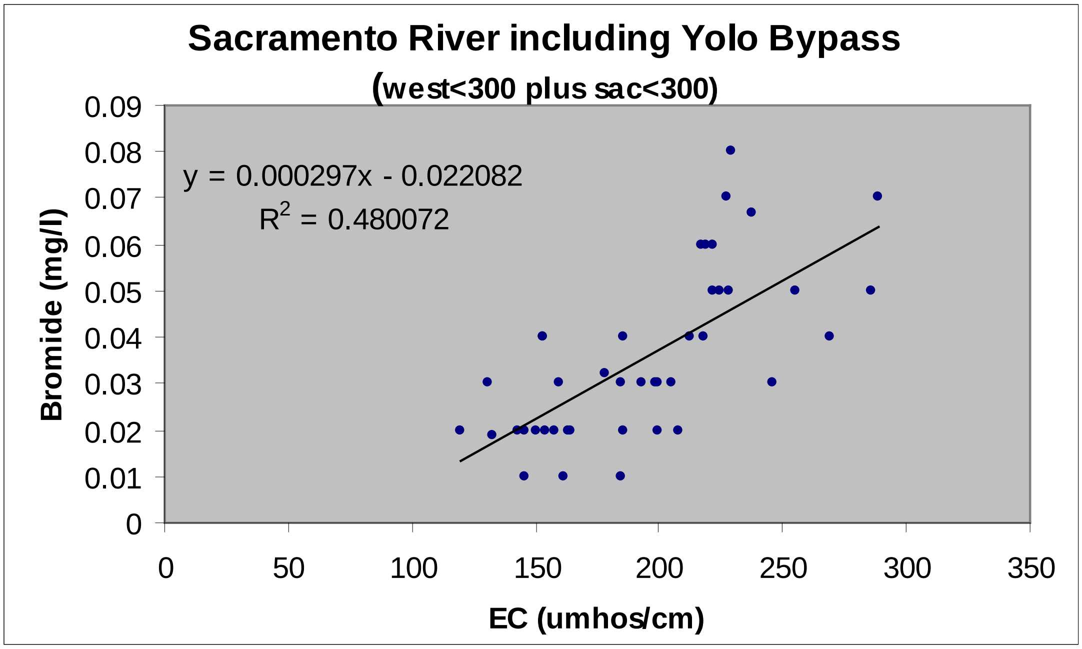


Figure 5-2 Sacramento River Boundary Regression Used for Converting from EC to Bromide

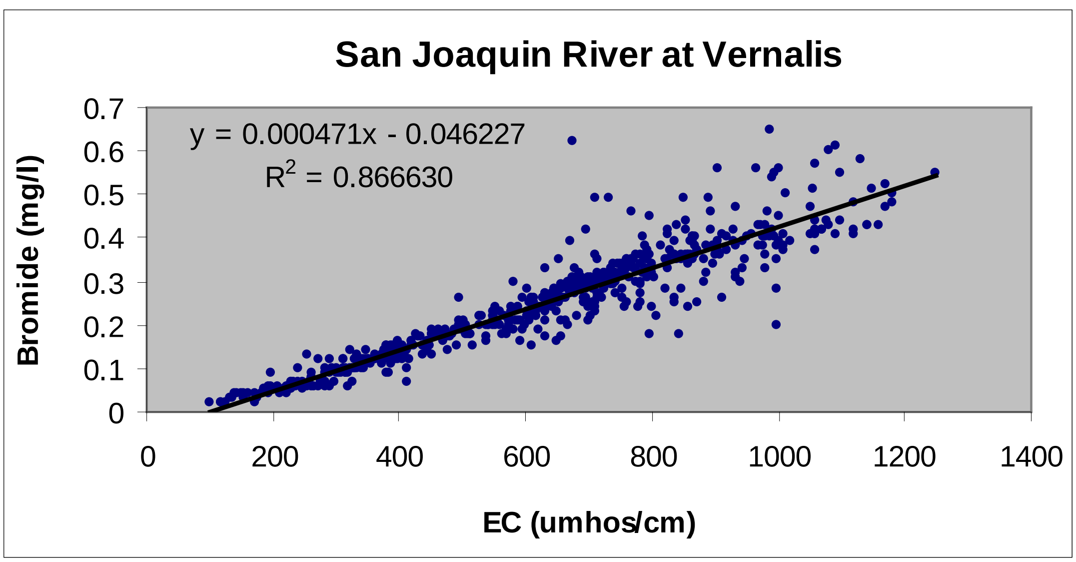


Figure 5-3 San Joaquin River Boundary Regression Used for Converting from EC to Bromide

Besides water quality at boundaries, DSM2 also requires that water quality for Delta island return flows be specified. Bromide data for Delta island return flows is scarce. Thus, in the current DSM2 bromide simulation, bromide data for Delta island return flows was based upon a memorandum report(California Department of Water Resources, 1995). The data was reported for 2 Delta regions shown (with lighter and darker shades) in Figure 5-4.

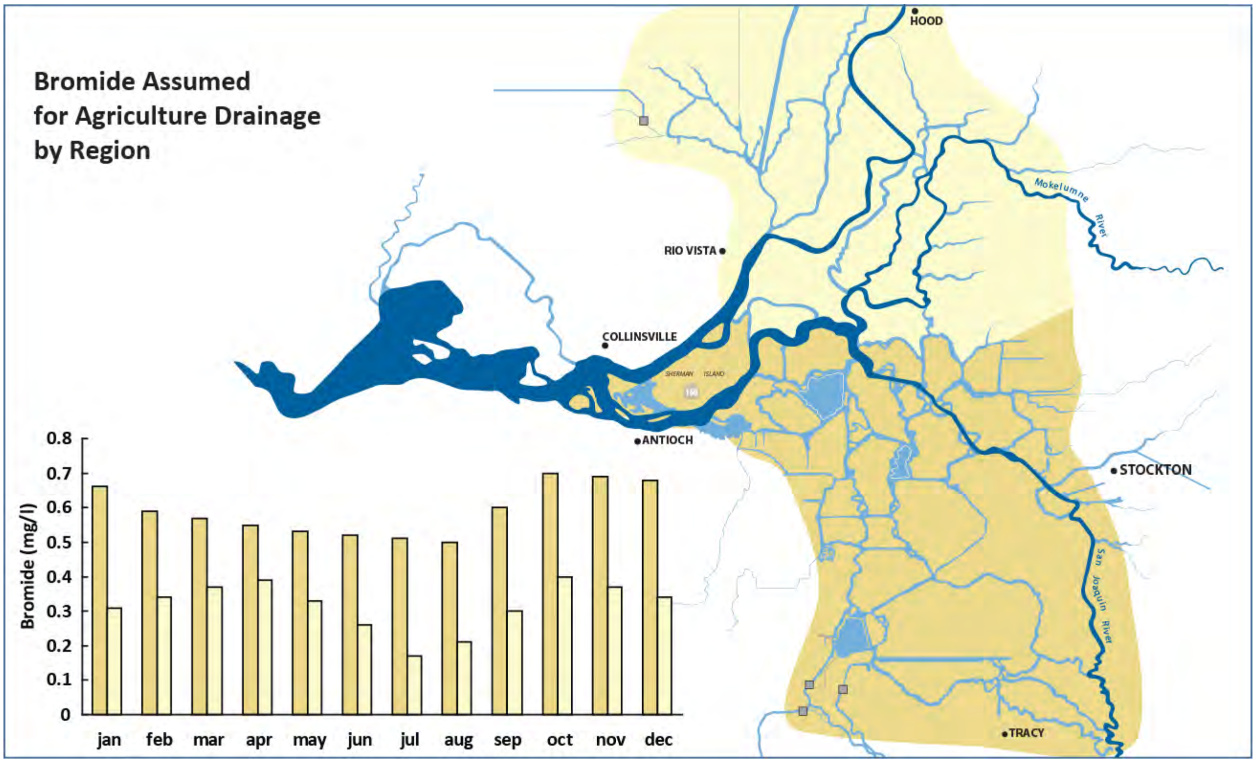


Figure 5-4 Bromide Assumed for Agricultural Drainage by Region

5.4 Estimating Historical Bromide Based on Simulated EC

Analysis in the past, based on grab sample EC and other constituents (bromide, chloride, magnesium, calcium, TDS, sulfide, total alkalinity, potassium, and sodium), has consistently shown certain patterns. At low EC values, the concentration of other constituents is bounded within a small range. But at higher EC values, the possible concentration of other constituents can vary over a larger range. The source of water when there are higher EC values will affect the percentage of bromide present in the concentration. For water from the ocean boundary, there will be a higher concentration of bromide. For water that is more influenced by the San Joaquin River or by Delta agricultural returns, the concentration of bromide will be lower, but the concentration of other constituents will be higher.

As shown in Figure 5-5, the concentration of a constituent can be bounded within two lines. This is the result of the complex mixing of water from different sources. Figure 5-5 shows two points with almost the same EC values but quite different bromide concentrations. The main graph shows a scatterplot between measured bromide and EC. A linear regression is made through the points and the R^2 value is 0.79, indicating that there is a spread in the data which becomes larger at greater EC and bromide levels. The two bar charts (fingerprints) show the makeup of EC and the percentage of water by volume from the different sources that contribute to Jones Pumping Plant water. At point 1, water from the Martinez boundary contributed most EC, so bromide concentration is high. At point 2, water from the San Joaquin

River contributed most EC, contribution from the Martinez boundary is negligible, and thus bromide concentration is much less.

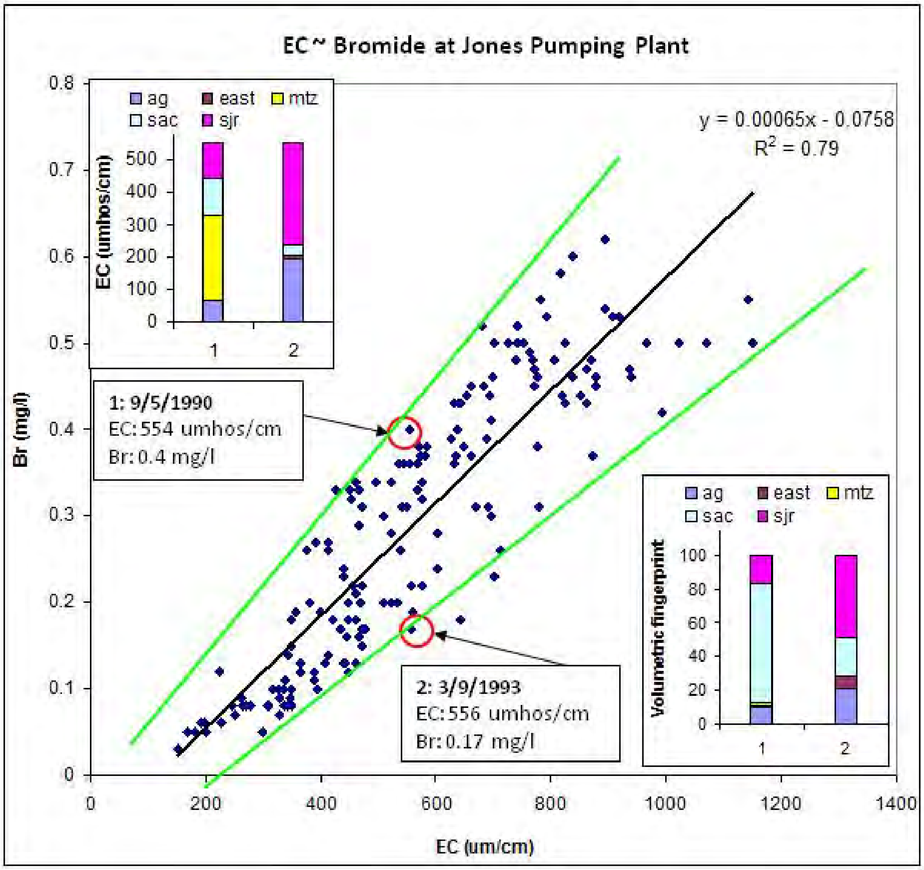


Figure 5-5 Illustration of Change of Bromide Concentration with Change of Water Sources

Based on the previous observation and the close EC-bromide relationship at boundaries, it is reasoned that it is very feasible that the bromide concentration at any location can be derived from the EC fingerprint of water from boundary sources. The following is the mathematical form that calculates bromide concentrations from EC fingerprints using multiple linear regressions,

$$Br = EC * (A*EC_{fp,mtz} + B*EC_{fp,sac} + C*EC_{fp,sjr} + D*EC_{fp,east} + E*EC_{fp,agr}) / EC_{all} \qquad \text{(Equation 2)}$$

where *Br* is the bromide concentration in mg/L; EC can be observed EC or modeled EC at a location; A, B, C, D, and E are coefficients; and $EC_{fp,mtz}$, $EC_{fp,sac}$, $EC_{fp,sjr}$, $EC_{fp,east}$, $EC_{fp,agr}$ are EC fingerprints at a specific location in the Delta from the 5 boundary sources: Martinez, Sacramento River, San Joaquin River, Eastside streams and Delta return flows. EC_{all} is total model simulated EC, i.e.,

$$EC_{all} = EC_{fp,mtz} + EC_{fp,sac} + EC_{fp,sjr} + EC_{fp,east} + EC_{fp,agr} \qquad \text{(Equation 3)}$$

Equation (2) can be re-organized as

$$Br = A*(EC*EC_{fp,mtz} / EC_{all}) + B*(EC*EC_{fp,sac} / EC_{all}) + C*(EC*EC_{fp,sjr} / EC_{all}) + D*(EC*EC_{fp,east} / EC_{all}) + E*(EC*EC_{fp,agr} / EC_{all}) = Br_{mtz} + Br_{sac} + Br_{sjr} + Br_{east} + Br_{agr} \quad \text{(Equation 4)}$$

Equation (4) indicates that bromide concentration at each specific location is the sum of bromide concentrations from each source. Thus multiple linear regressions can be used to estimate not only total bromide concentrations, but also bromide fingerprints.

A multiple linear regression can be developed for different regional scales. It can be developed using all grab sample data available within the Delta so a Delta-wide regression can be obtained, in which case, one set of coefficients can be used for all stations in the Delta. It can also be conducted for each station using limited data at that station so there will be a set of coefficients for each site-specific regression.

Without doubt, best results can be achieved by using the site-specific regression approach. However, this can only be done for locations with grab sample data. For locations without grab sample data, it is difficult to use this approach. The Delta-wide regression is elegant and the simplest, but at the cost of sacrificing accuracy for some locations.

Several years ago, BDO analyzed EC and bromide relationships [(Suits, 2001), (Suits, 2002), (Hutton, 2006)]. It was found that a close relationship between EC and bromide exists for boundary locations and all stations in the Delta. Further study indicated that it is not necessary to have a regression for each single station. Instead, several stations may have characteristics in common and can be grouped to form a region; and as a result, a regression will apply to all locations within the region.

Figure 5-6 is a map of the regions that were defined based on available grab sample locations. It is anticipated that by grouping stations into regions, accuracy at each station can be maintained with regressions only conducted for regions. Therefore, the number of regressions is reduced considerably compared with the number of site-specific regressions.

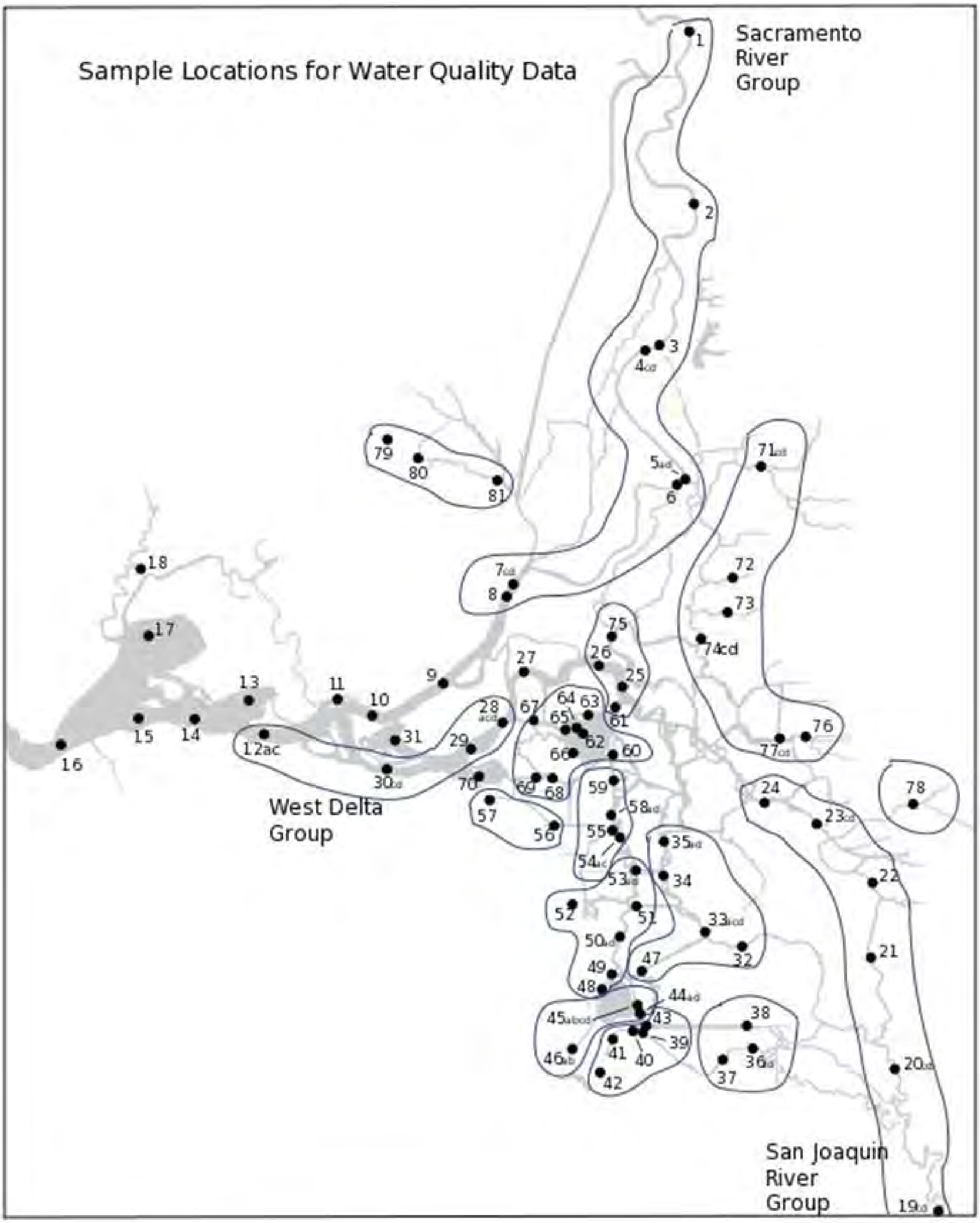


Figure 5-6 Grab Sample Locations and Groupings for Derivation of Regressions

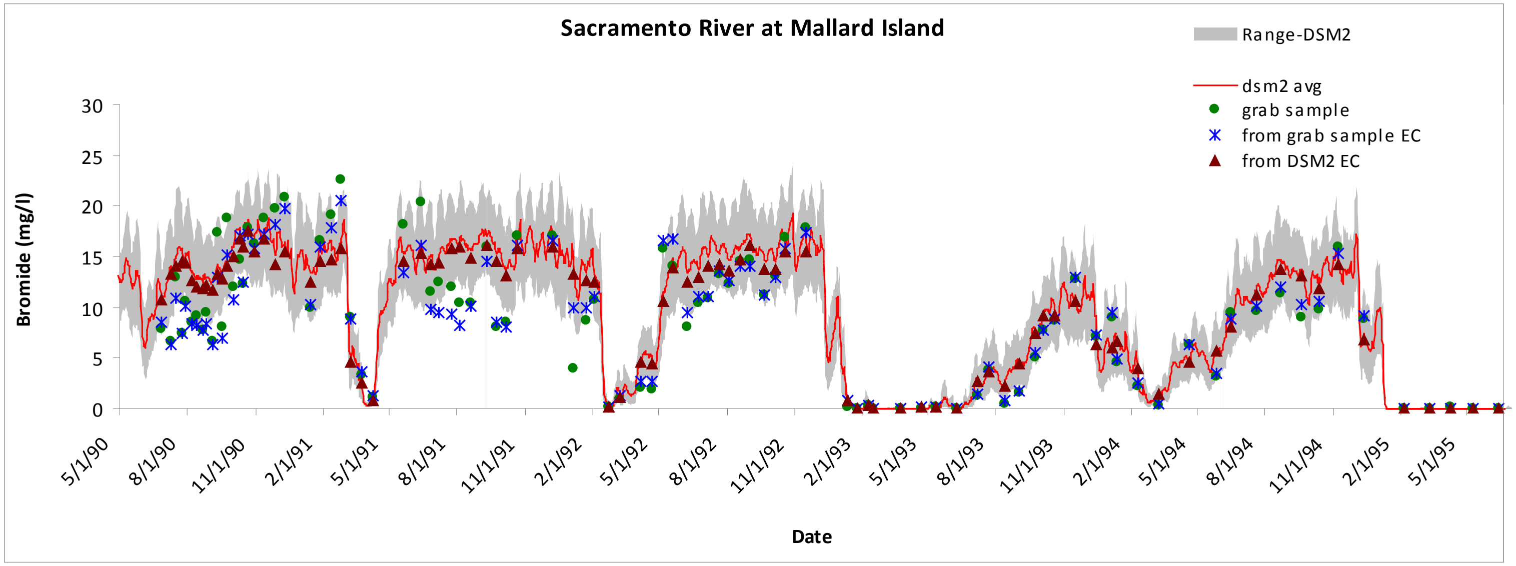
5.5 Comparison of Direct Bromide Simulation and Delta-wide Regression

Figure 5-7 through Figure 5-12 show the following:

- Grab sample bromide (observed)
- DSM2 modeled bromide (direct simulation)
- DSM2 modeled EC and then converted to bromide using a Delta-wide multiple linear regression
- Grab sample (observed) EC converted to bromide using a Delta-wide multiple linear regression

Because the bromide concentration can vary a lot within one day, the graphs also show the range of bromide values for each day. For Jones Pumping Plant and the Sacramento River at Mallard Island, the ranges can be seen clearly. For other locations, the changes of bromide concentration within a day are not significant.

From the figures, we can see that most of the time the grab sample bromide concentrations (green, filled circles) fall within or close to the bromide range simulated by DSM2 (gray area). Bromide concentrations estimated by using the multiple linear regression that used EC fingerprint and DSM2-simulated EC (red triangles) are very close to DSM2-calculated bromide concentrations (gray area). This is anticipated because the bromide concentrations at boundaries were estimated using linear regressions between bromide and EC. However, better results can be obtained by using a multiple linear regression and grab sample EC (blue asterisks), which better matches the grab sample bromide concentrations (overall the blue asterisks are nearer to the green circles). It is apparent that this approach can decrease errors caused by the limitations of the DSM2 model. A comparison of the different methods of determining bromide is analyzed mathematically following the figures.



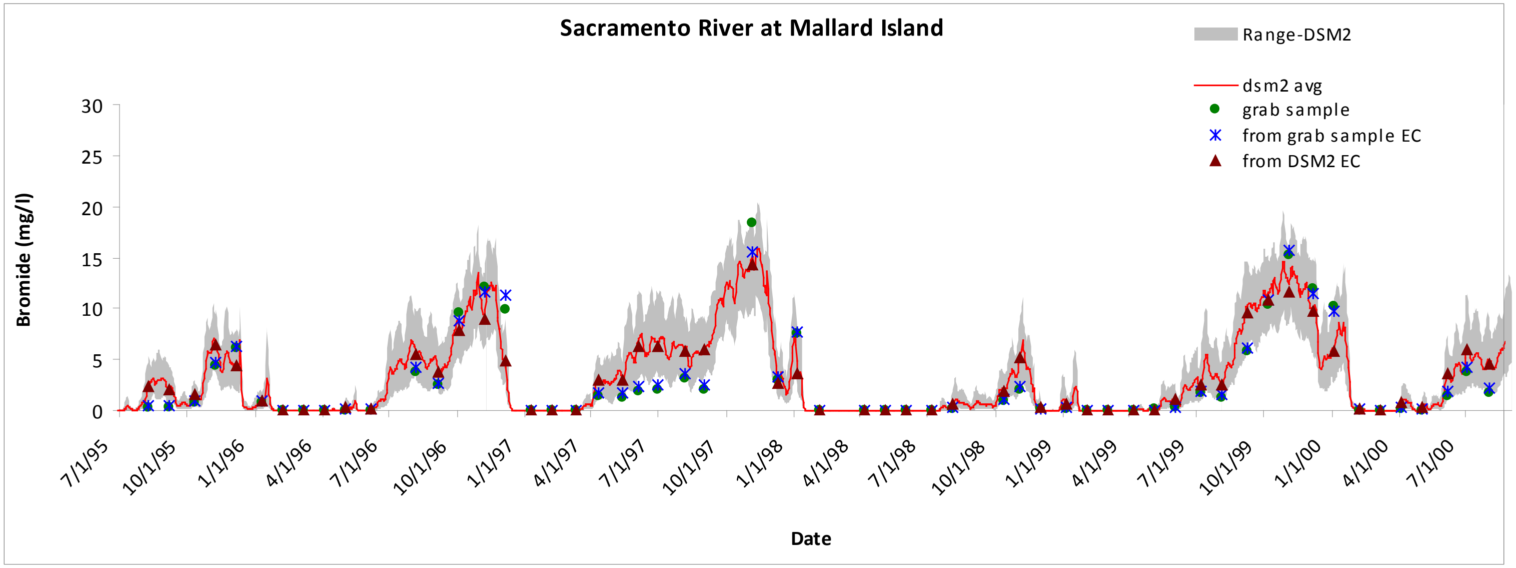
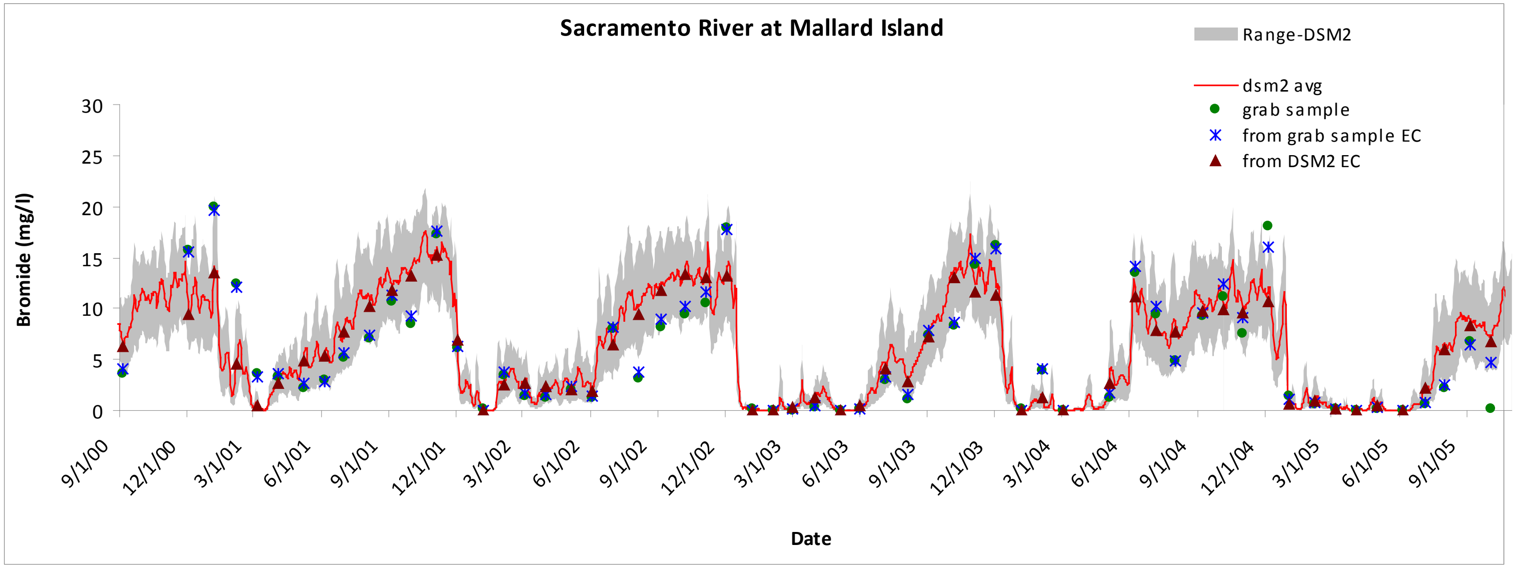


Figure 5-7 Comparison of Grab Sample Data and Calculated Bromide Concentration at Sacramento River at Mallard Island (four figures total)



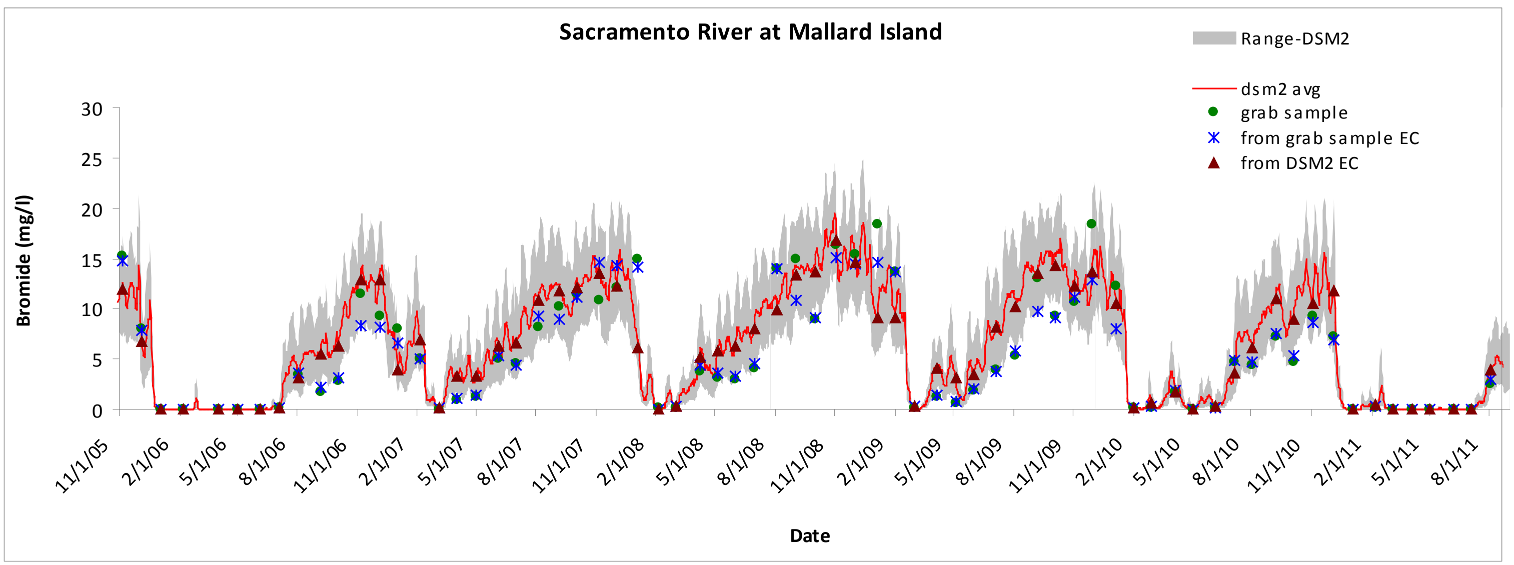
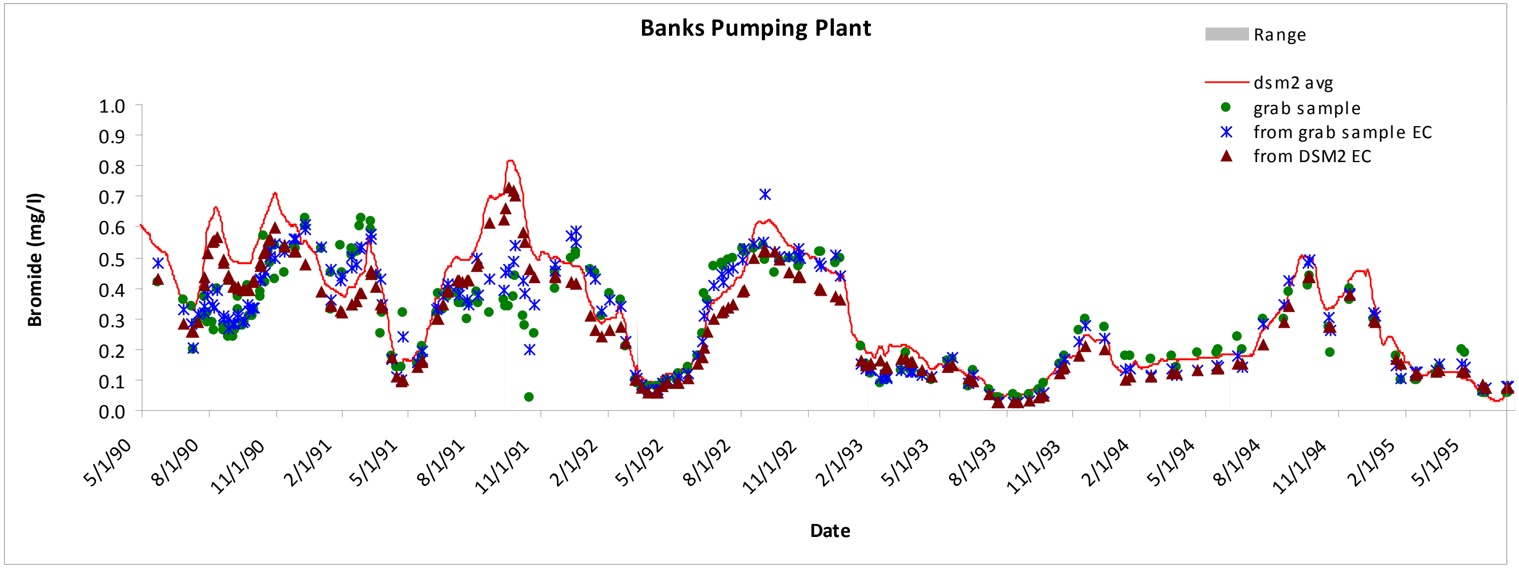


Figure 5 7 (cont'd) Comparison of Grab Sample Data and Calculated Bromide Concentration at Sacramento River at Mallard Island



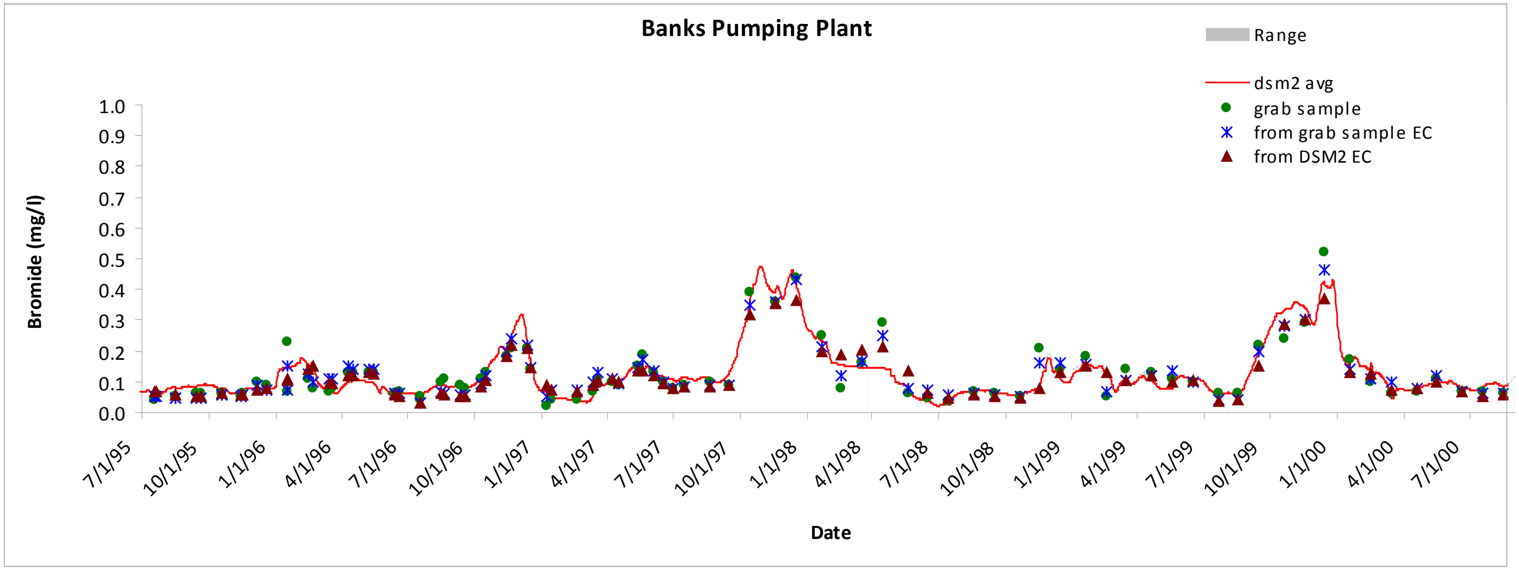
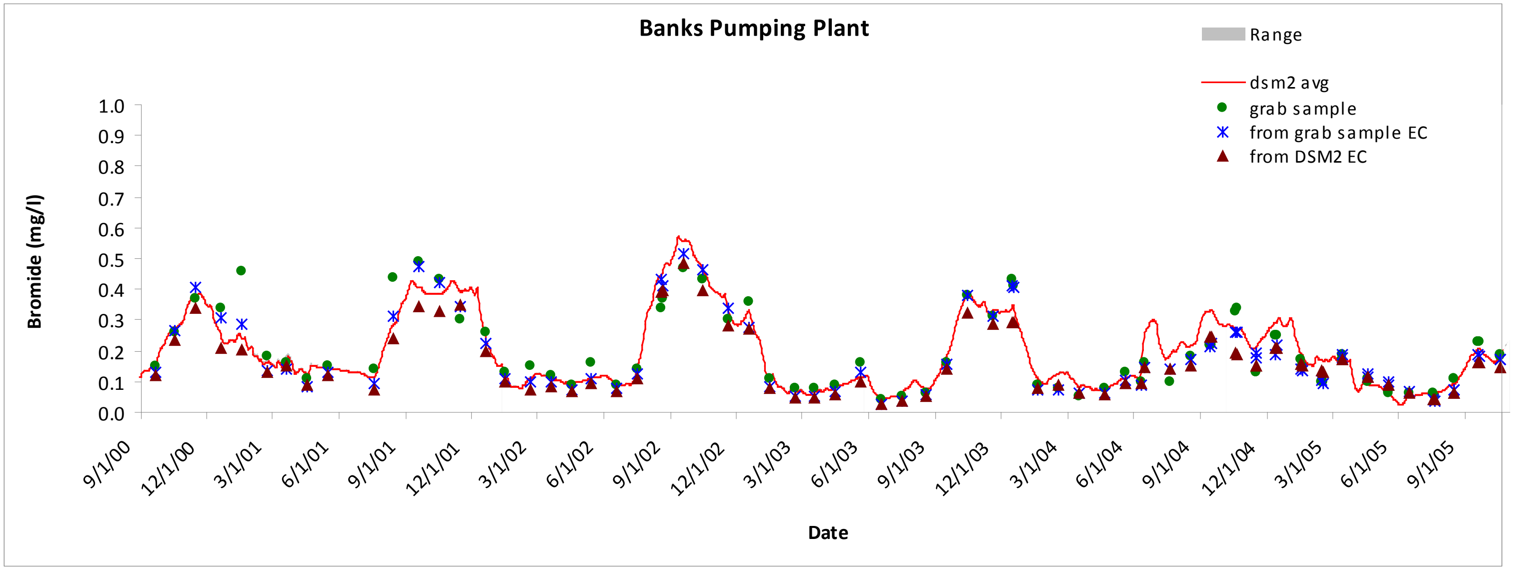


Figure 5-8 Comparison of Grab Sample Data and Calculated Bromide Concentration at Banks Pumping Plant (four figures total)



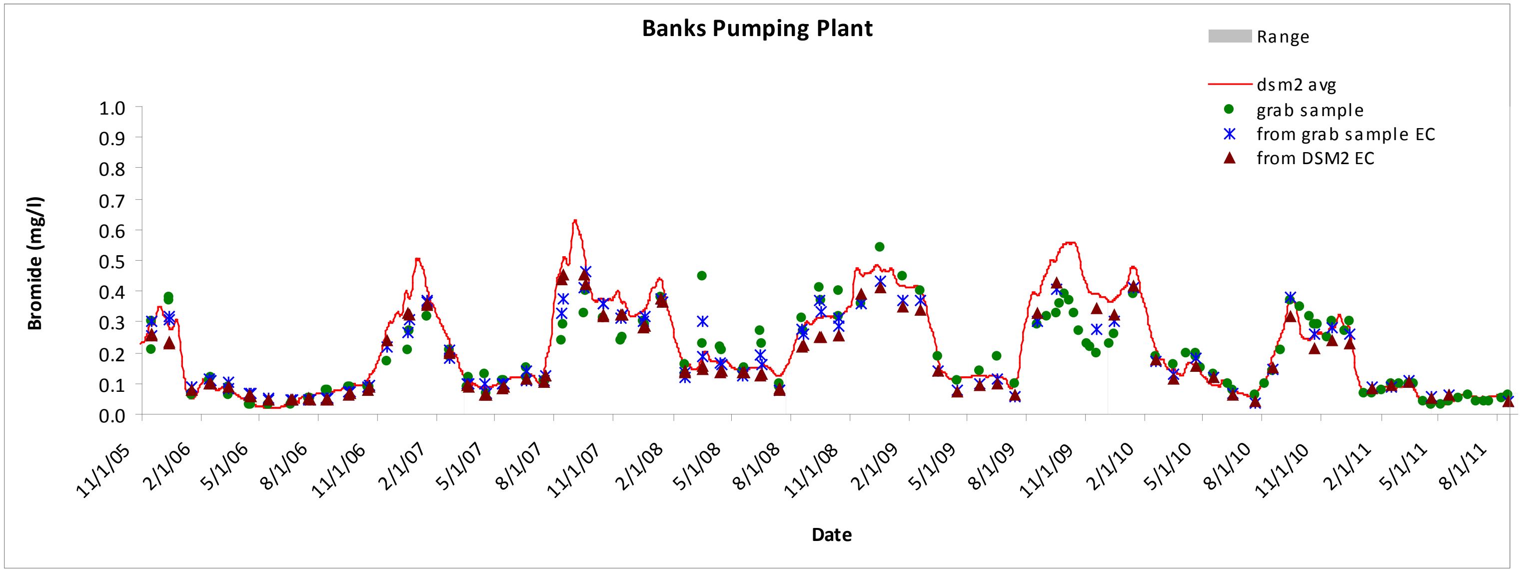
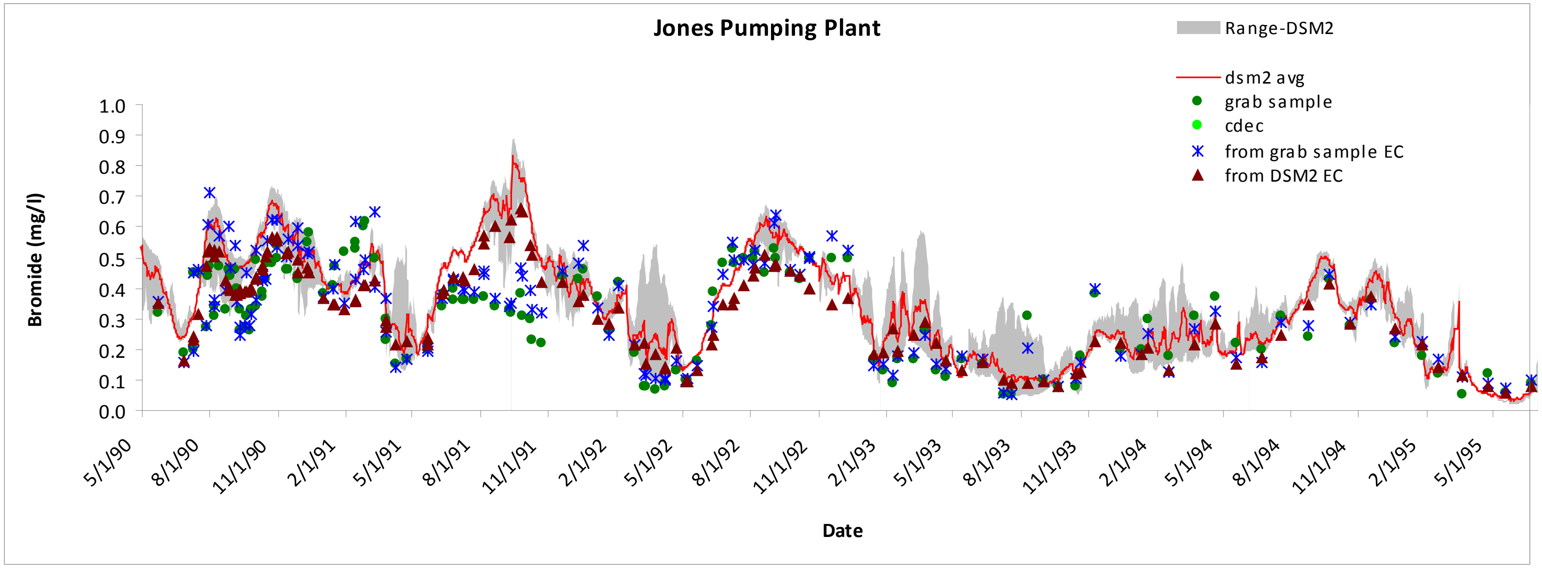


Figure 5-8 (cont'd) Comparison of Grab Sample Data and Calculated Bromide Concentration at Banks Pumping Plant



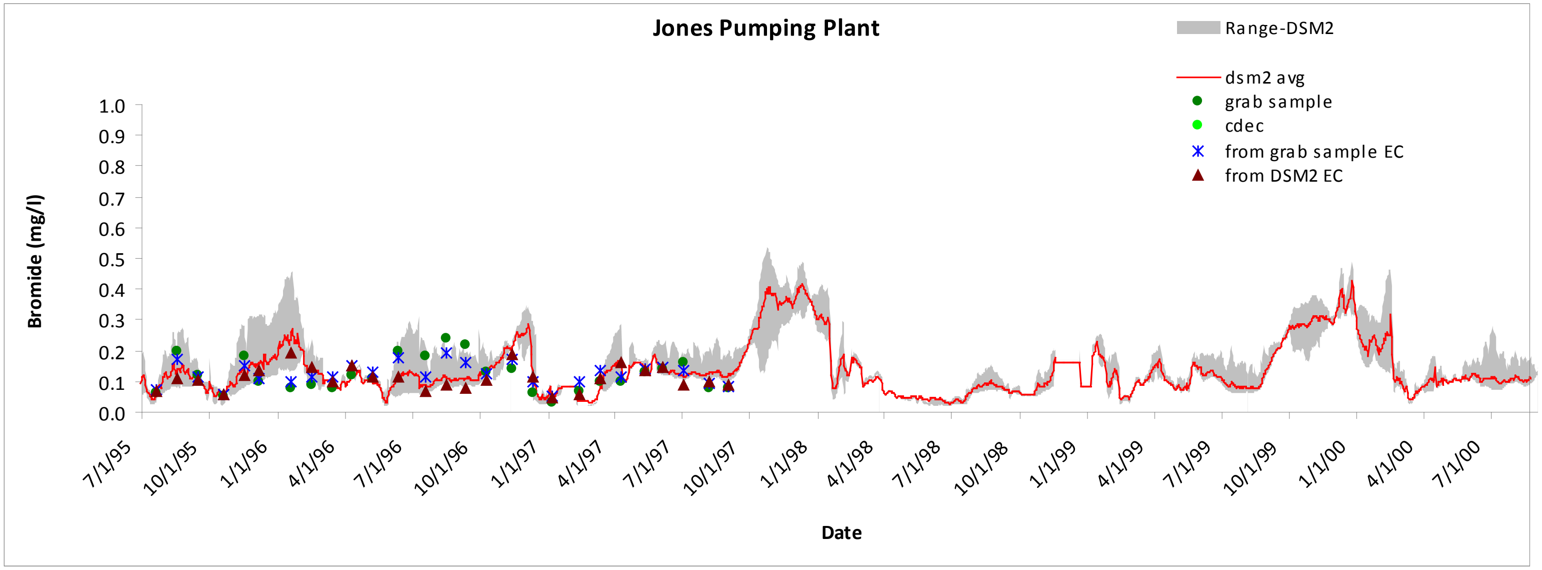
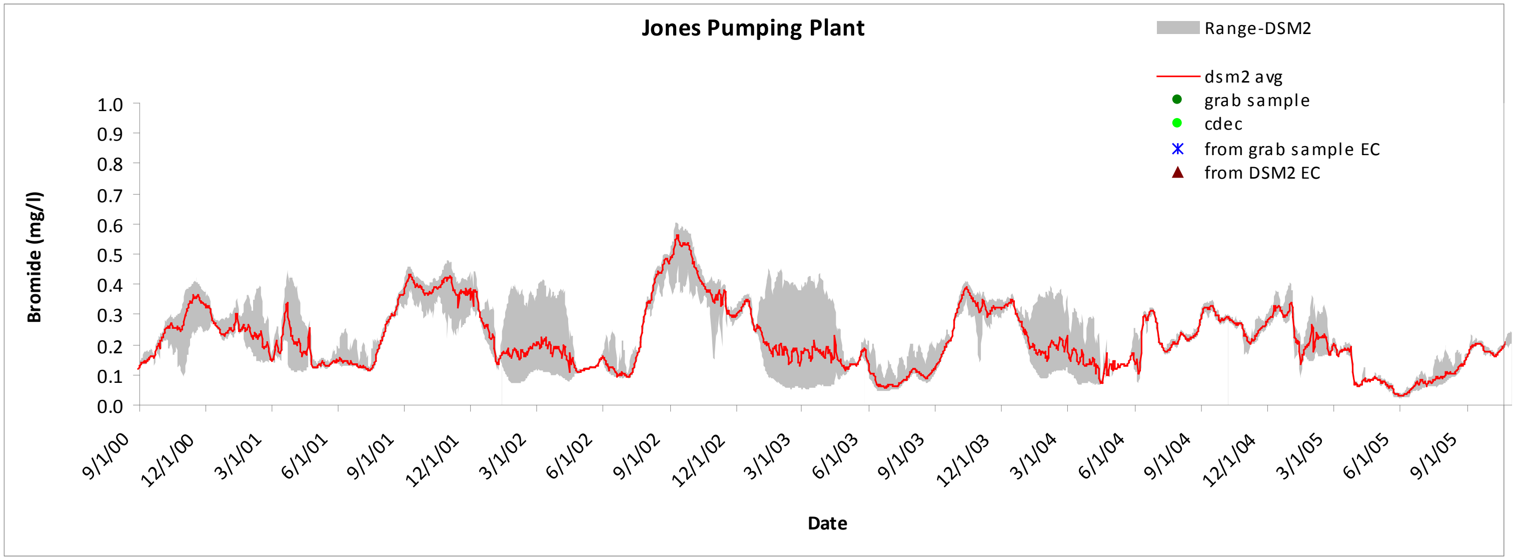


Figure 5-9 Comparison of Grab Sample Data and Calculated Bromide Concentration at Jones Pumping Plant (four figures total)



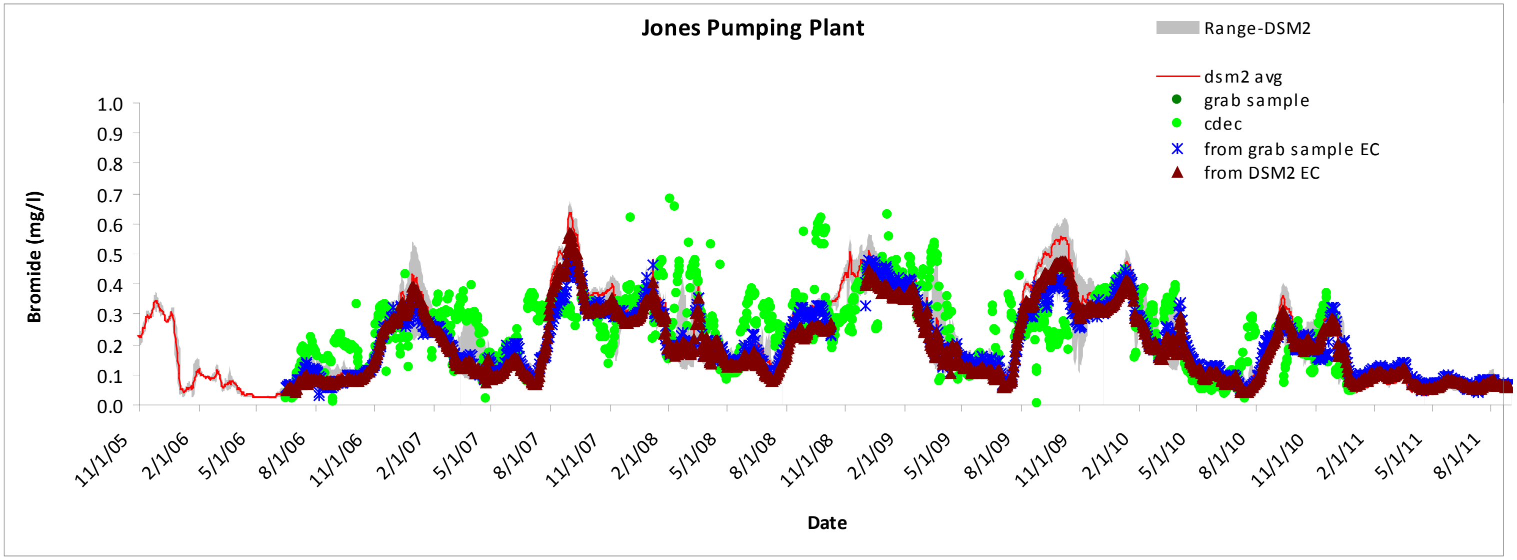
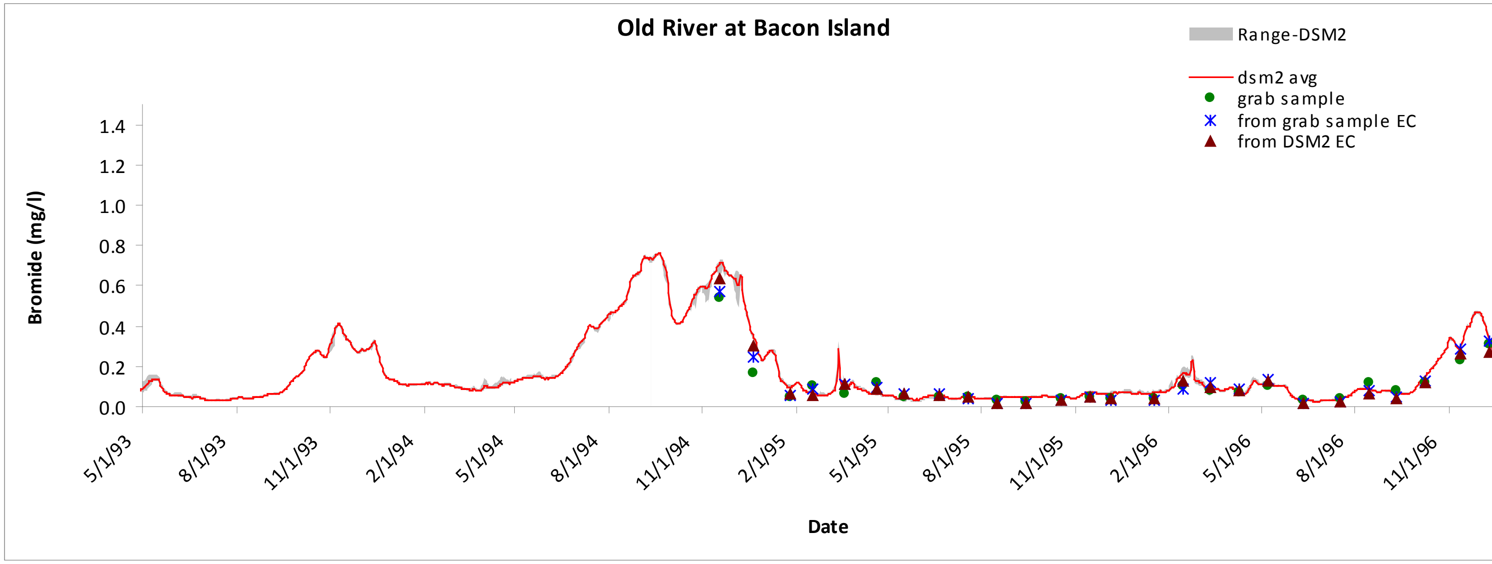


Figure 5-9 (cont'd) Comparison of Grab Sample Data and Calculated Bromide Concentration at Jones Pumping Plant



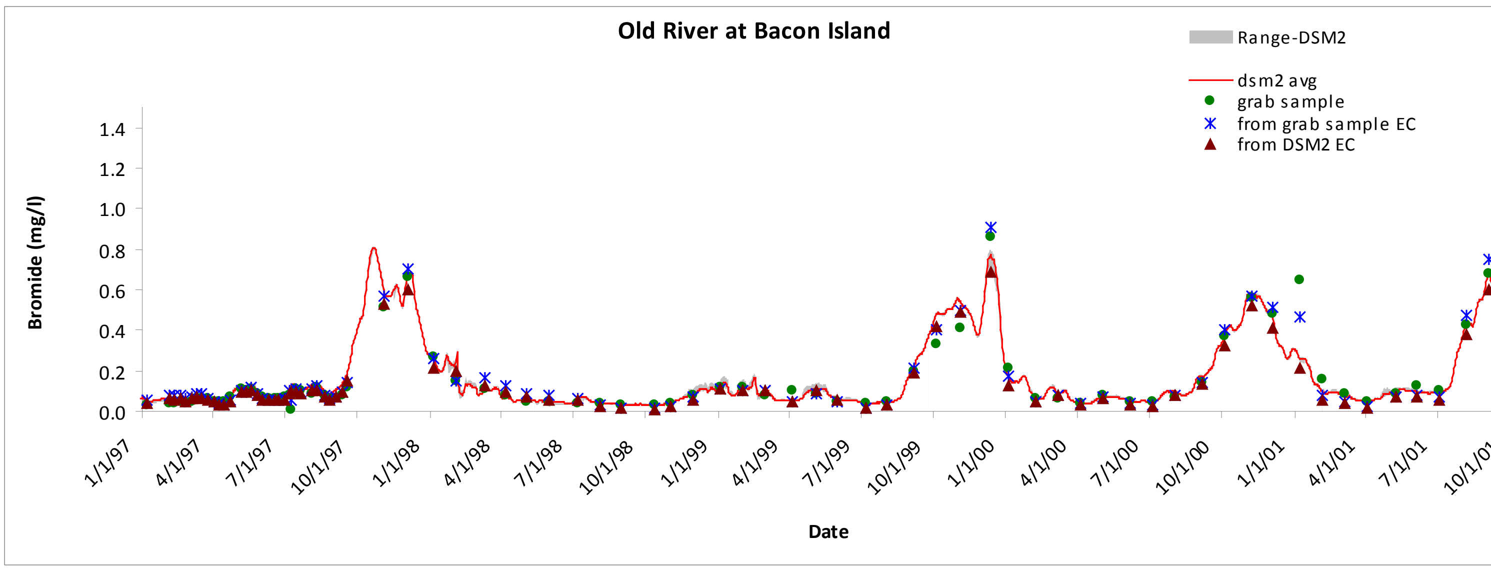
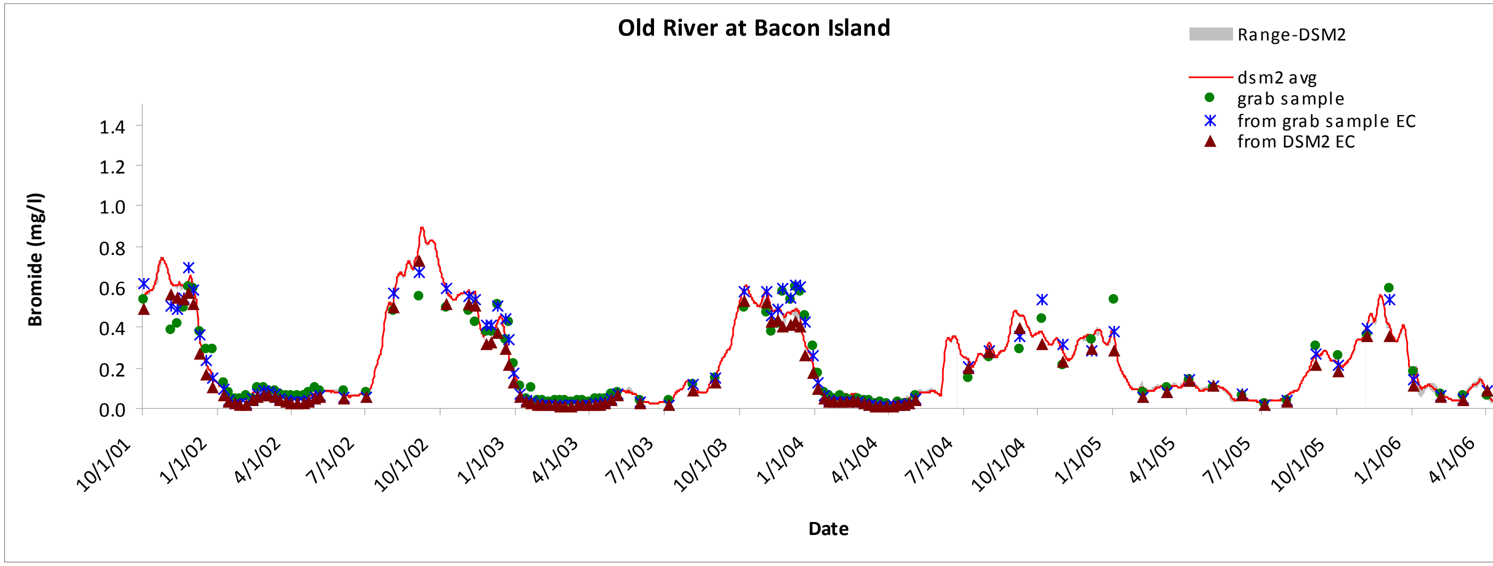


Figure 5-10 Comparison of Grab Sample Data and Calculated Bromide Concentration in Old River at Bacon Island (four figures total)



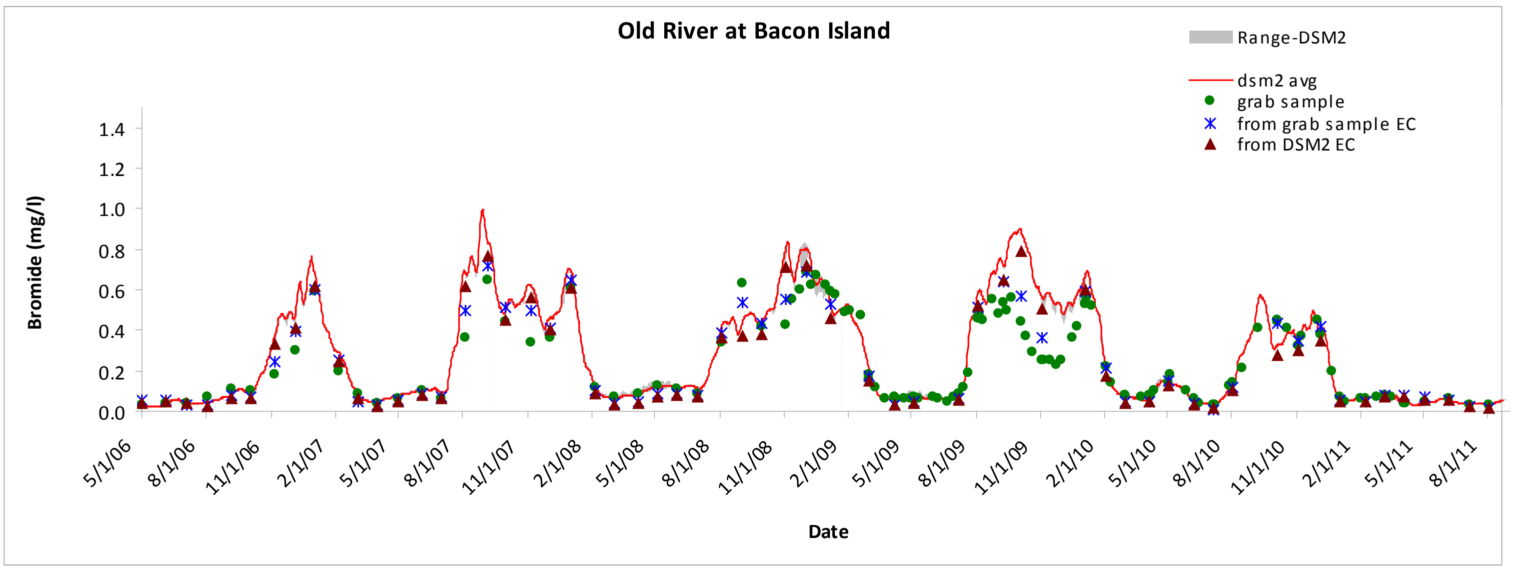
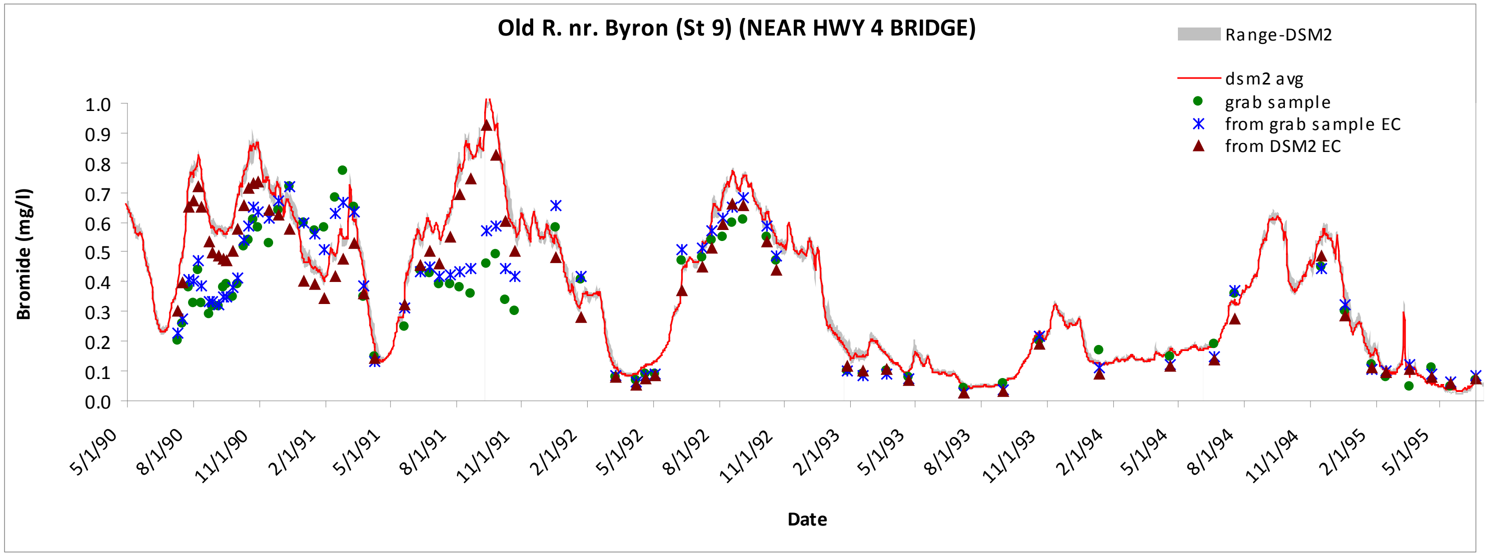


Figure 5-10 (cont'd) Comparison of Grab Sample Data and Calculated Bromide Concentration in Old River at Bacon Island



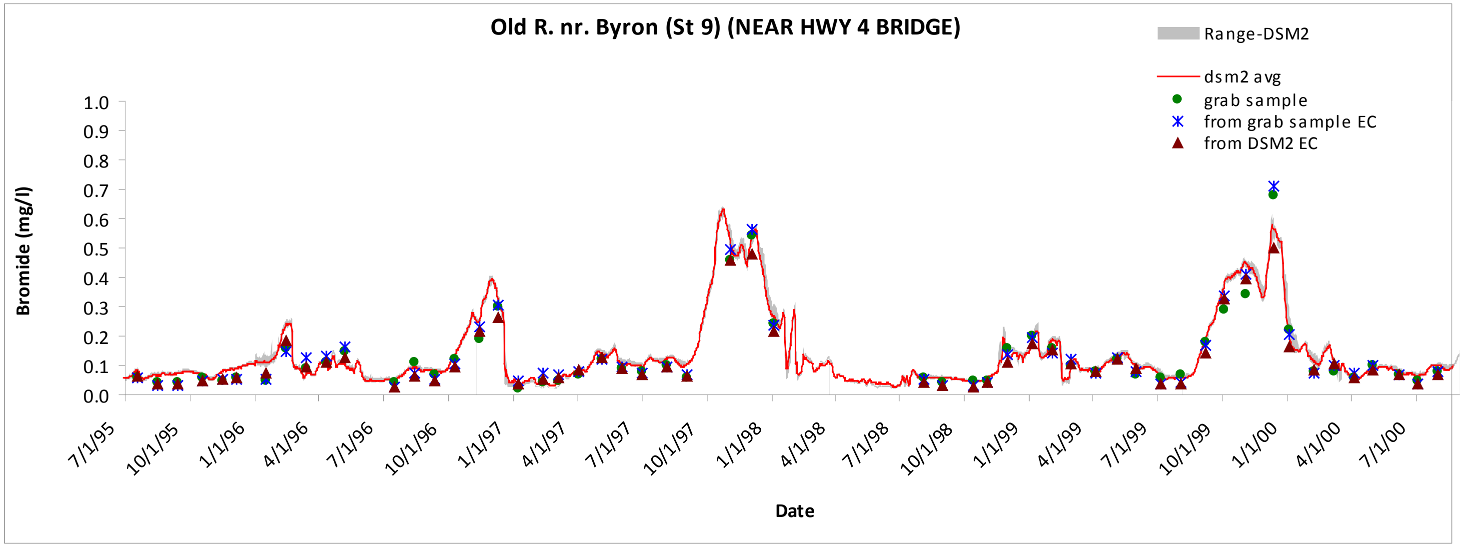
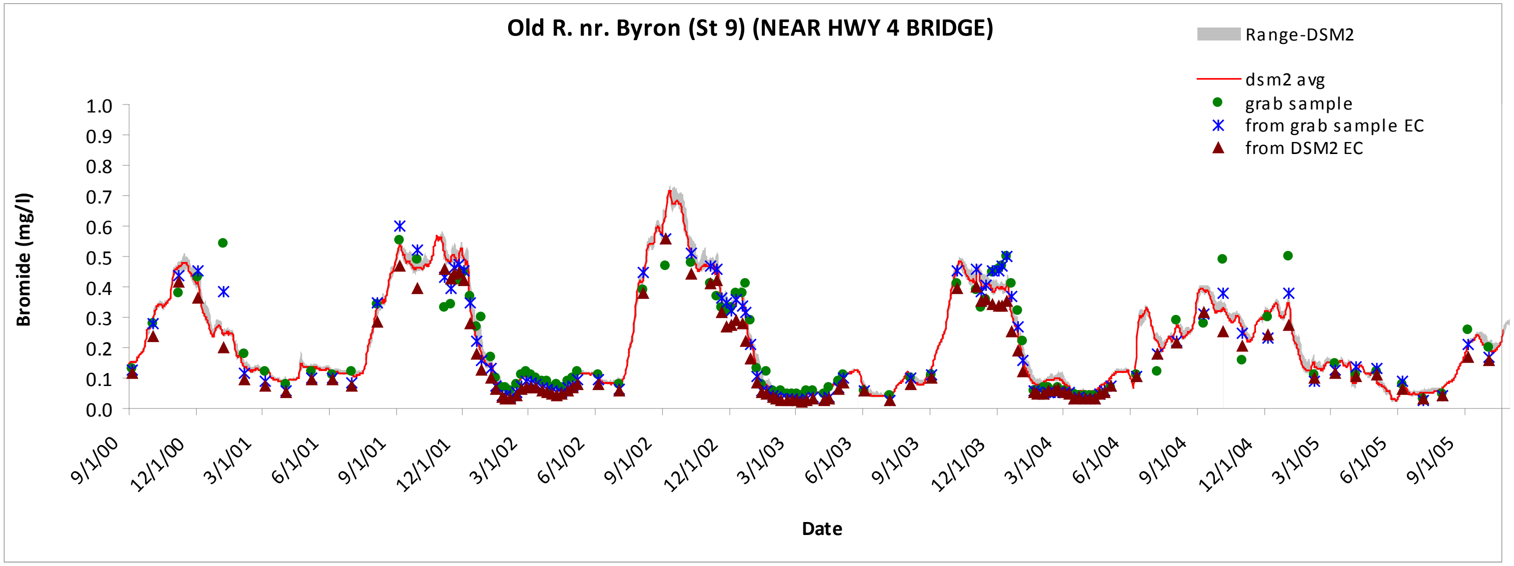


Figure 5-11 Comparison of Grab Sample Data and Calculated Bromide Concentration in Old River near Highway 4 Bridge (four figures total)



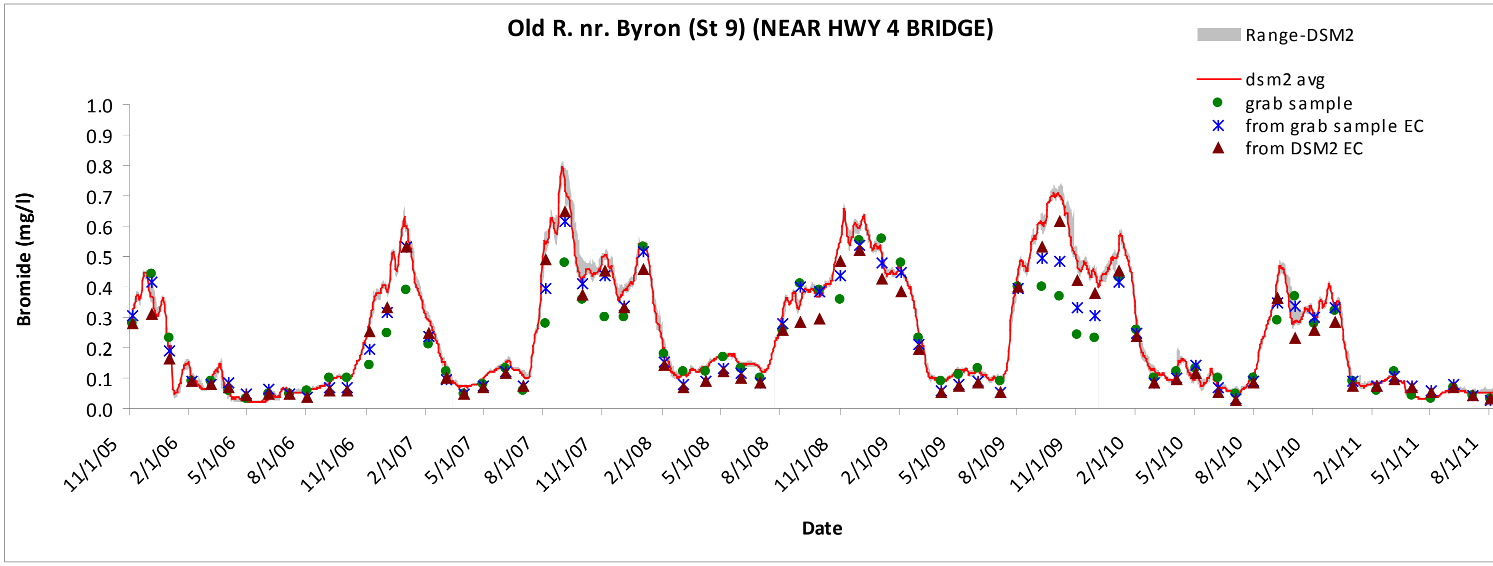
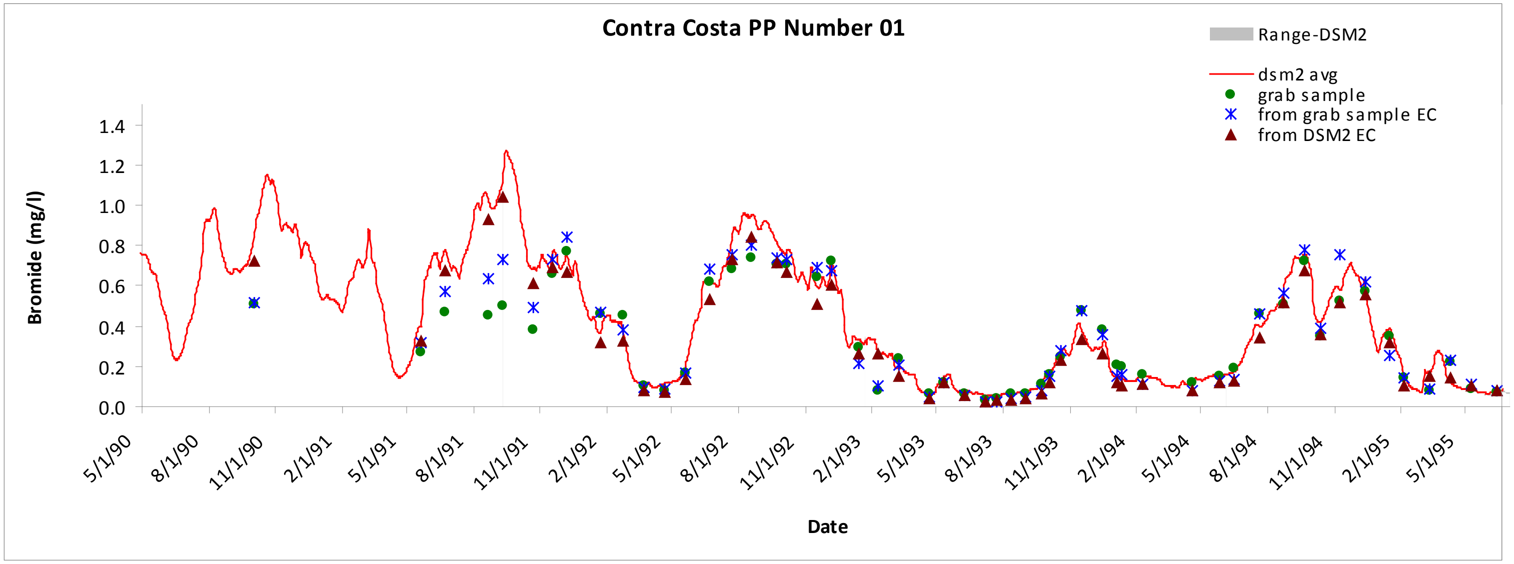


Figure 5-11 (cont'd) Comparison of Grab Sample Data and Calculated Bromide Concentration in Old River near Highway 4 Bridge



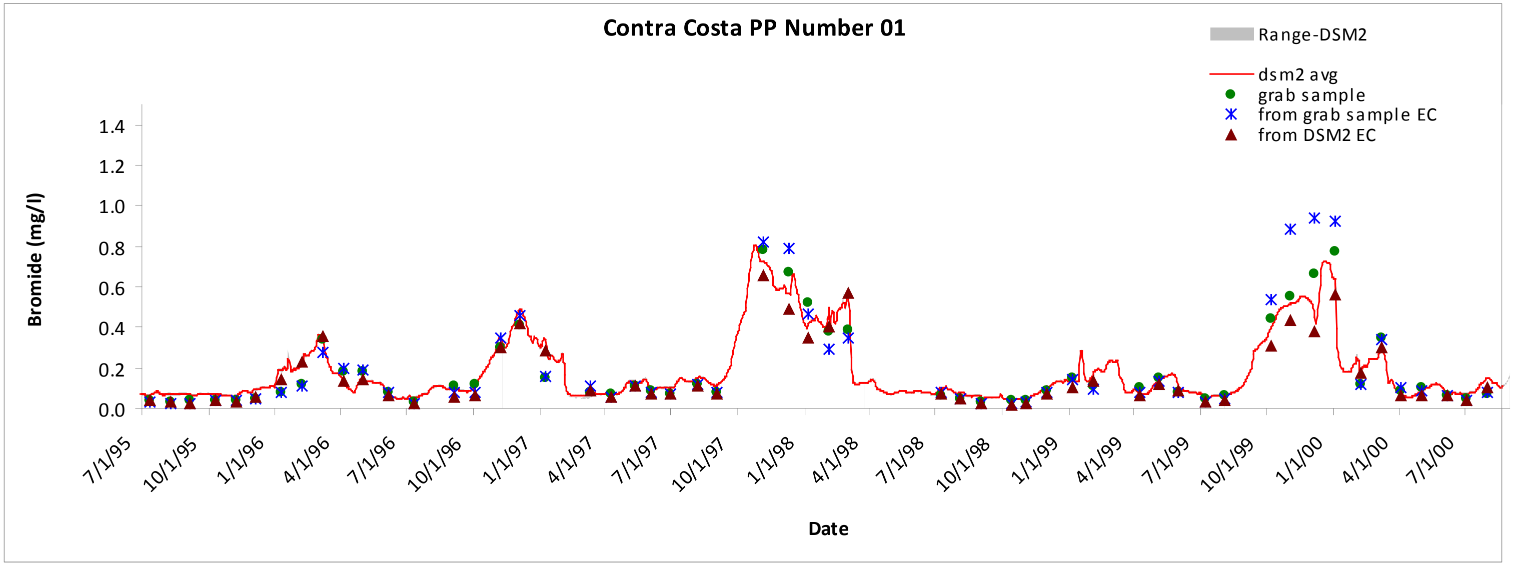
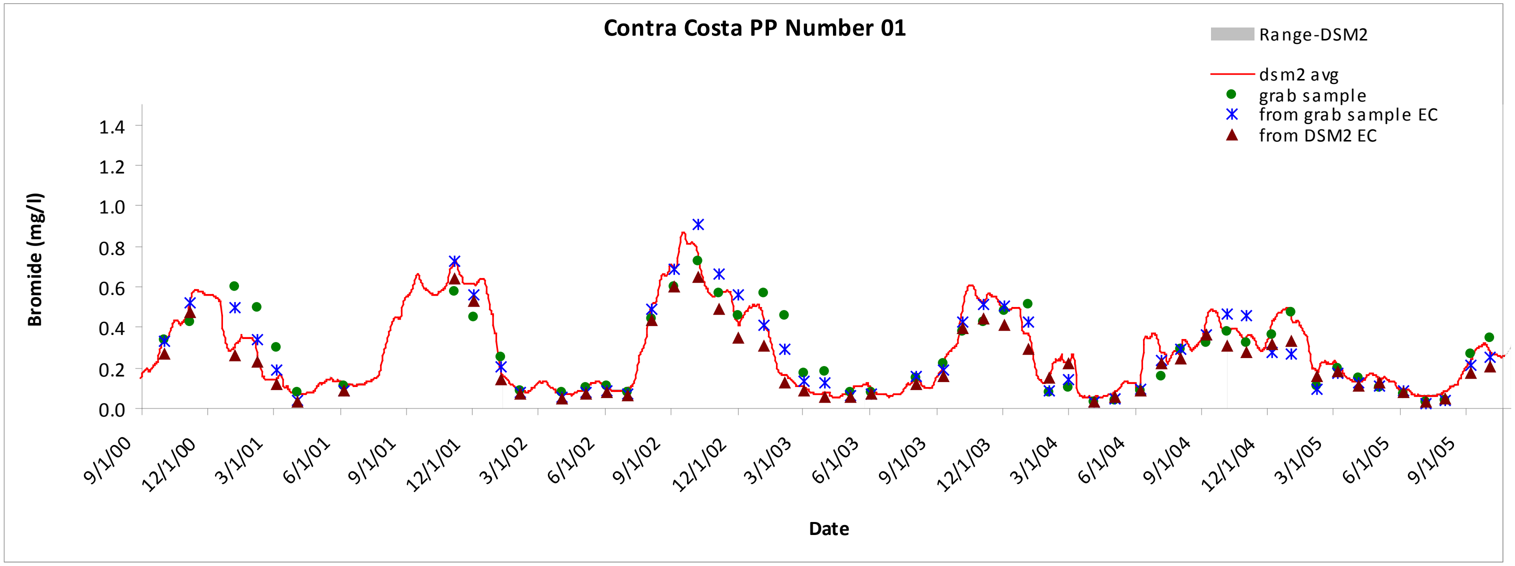


Figure 5-12 Comparison of Grab Sample Data and Calculated Bromide Concentration at Contra Costa Pumping Plant 1 (four figures total)



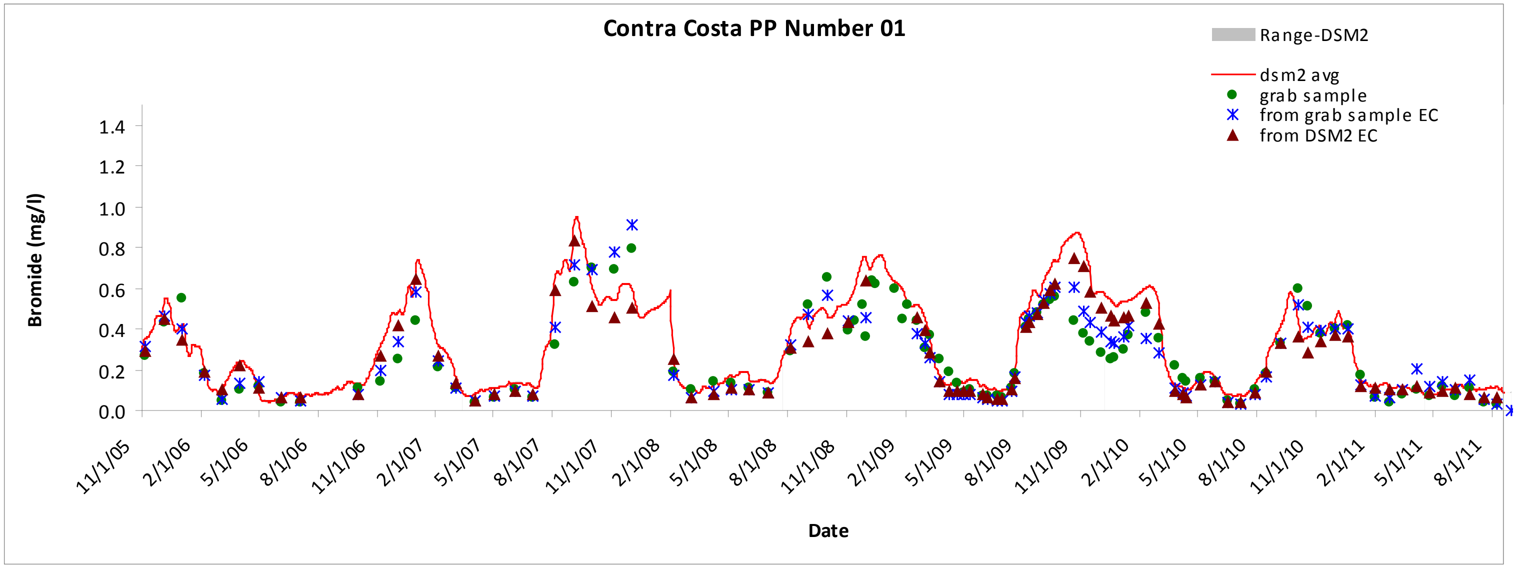


Figure 5-12 (cont'd) Comparison of Grab Sample Data and Calculated Bromide Concentration at Contra Costa Pumping Plant 1

5.6 Comparison of Performance of Different Methods in Estimating Bromide

To compare the performance of each method, the Nash–Sutcliffe model efficiency coefficient is used. It is defined as

$$E = 1 - \frac{\sum_{t=1}^{T}(Q_o^t - Q_m^t)^2}{\sum_{t=1}^{T}(Q_o^t - \overline{Q_o})^2} \quad \text{(Equation 5)}$$

where E is the Nash–Sutcliffe model efficiency coefficient; Q_o^t is observed value at time *t;* Q_m^t is model calculated value at time *t;* and $\overline{Q_o}$ is the average of the observed values.

Nash–Sutcliffe (N-S) efficiencies can range from −∞ to 1. An efficiency of 1 ($E = 1$) corresponds to a perfect match of estimated bromide to the observed data. An efficiency of 0 ($E = 0$) indicates that the model predictions are as accurate as the mean of the observed data, whereas an efficiency less than zero ($E < 0$) occurs when the observed mean is a better predictor than the model (Wikipedia, 2011).

Table 5-2 is a summary of the N-S efficiencies estimated from 6 methods at 17 grab sample locations. The first column shows all the stations used in this study for comparison of different methods. Column 2 lists N-S efficiencies from direct DSM2 simulation. It must be pointed out that the daily bromide values from DSM2 output were used to calculate the N-S efficiencies, but grab sample bromide concentrations are instantaneous values. So the actual N-S efficiencies for DSM2 simulation may be better than those listed in the table. Column 3 lists N-S efficiencies from direct EC ~ bromide regression. The site-specific regression did not consider the fingerprint of each source.

Column 4 lists N-S efficiencies from a regression developed in BDO in the past (Hutton, 2006) using equation (6). The regression was developed mainly for Banks Pumping Plant. However, in this memorandum, it was also used to calculate N-S efficiencies at other locations to see how it does at locations other than Banks Pumping Plant. The method consists of 2 expressions for 2 cases, corresponding to the condition that Martinez volumetric fingerprint at a location is more or less than 0.4%, the following are the 2 expressions,

$$Br = \begin{cases} -0.0364 + 0.0004 * EC & Vol_{MTZ} < 0.4 \\ -0.1117 + 0.0000827 * EC & Vol_{MTZ} > 0.4 \end{cases} \quad \text{(Equation 6)}$$

In columns 5, 6, and 7 are N-S efficiencies from multiple linear regressions that use EC fingerprint and grab sample EC. The difference is that different data sets were used in regression. For site-specific regression, only grab sample data at a location was used to get regression coefficients. For regional regression, grab sample data at all locations within a region was used to get regression coefficients for that region; and the same coefficients were used for all locations within the region. For Delta-wide regression, all grab sample data at locations within the Delta was used to get regression coefficients; and the same coefficients were used for all locations.

It is true that the N-S efficiencies for direct bromide DSM2 simulation may be underestimated because daily values of bromide calculated by DSM2 were compared against grab sample bromide data. But it is not expected that N-S efficiencies for direct DSM2 bromide simulation at Banks and Jones Pumping Plants are greater than 0.8 because the N-S efficiencies for direct EC simulation at Banks and Jones Pumping Plants are 0.72 and 0.76 respectively, based on historical EC simulation from January 1, 1990, to August 31, 2011. It is assumed that the N-S efficiencies for bromide simulation will be quite similar to the N-S efficiencies for EC simulation.

As expected, the site-specific regression did the best for all locations. The direct EC-bromide regression did very well for some locations, but not so well for other locations. Surprisingly, the previous BDO regression did well for a lot of locations including Banks Pumping Plant, Contra Costa Pumping Plant, and Old River at Bacon Island. Without doubt, Delta-wide regression did better than direct EC ~ bromide regression, especially for such locations as Banks Pumping Plant, Jones Pumping Plant, and Contra Costa Pumping Plant. The regional regression performed almost as well as the site-specific regression, but can be used more conveniently.

Table 5-2 Comparison of Performance of Different Methods in Estimating Bromide

Grab sample locations	Direct EC-Br Regression (2)	Previous BDO Regression (3)	Site-specific Regression (4)	Regional Regression (5)	Delta-wide Regression (6)
SJRJERSEY	0.89	0.80	0.92	0.91	0.87
MALLARD	0.97	0.80	0.96	0.96	0.96
BANKS	0.87	0.94	0.95	0.95	0.93
DMC	0.79	0.77	0.91	0.91	0.86
MRIVBACON	0.75	0.88	0.92	0.91	0.87
MIDDLER	0.83	0.94	0.93	0.93	0.92
GRANTOLD	0.71	0.33	0.84	0.83	0.77
FALSETIP-WEBB	0.94	0.85	0.95	0.95	0.90
NORTHCAN	0.85	0.89	0.92	0.91	0.89
NVICWOOD	0.90	0.93	0.94	0.92	0.93
OLDRIVBACISL	0.96	0.97	0.98	0.98	0.95
ROCKSL	0.95	0.91	0.97	0.97	0.93
SANDMOUND	0.95	0.90	0.96	0.96	0.87
SANTAFEBACON	0.92	0.92	0.94	0.93	0.93
STATION09	0.94	0.97	0.97	0.97	0.94
STATION04B	0.95	0.89	0.97	0.96	0.93
CONCOSPP1	0.85	0.92	0.95	0.94	0.90

Table note: Numbers 2, 3, 4, 5, and 6 in column heads refer to method numbers as shown in Table 5-1. A number shown in gray box is the highest N-S value for that grab sample location.

5.7 Conclusions

Based on the comparison of grab sample data, modeling results, and calculated bromide concentrations, the following conclusions can be made:

1. BDO confirmed MWH's conclusion that the DSM2 model performs equally well in simulating bromide concentrations in the Delta as it does in modeling EC.
2. Delta-wide multiple linear regression based on EC fingerprints and DSM2-calculated EC performs as well as direct bromide simulation using DSM2.
3. Overall, Delta-wide multiple linear regression based on EC fingerprints and grab sample EC performs better than direct bromide simulation using DSM2.
4. Site-specific multiple linear regression performs the best at all locations. However, this approach cannot be used for locations without both measured bromide and EC data.
5. Regional multiple linear regression has close performance as site-specific regression, and can be used for locations without measured bromide data.
6. Multi-variable regression can be used to fingerprint bromide from each source.

5.8 References

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