

# Technical Memorandum

Date: 5/14/2010

To:	Paul Hutton, Metropolitan Water District
From:	Michael L. Deas, Watercourse Engineering, Inc.
Re:	Review of: Modeling the Fate and Transport of Ammonia Using DSM2- QUAL – Draft Final report (October 2009)

# Scope

The scope of work identified that the general purpose of the DSM2-QUAL review process was to address immediate questions that many stakeholders have – can the module be credibly applied to evaluate nutrient source-response relationships in the Delta under current conditions and under a variety of flow and load modification scenarios? Further guidance in the scope included specific questions:

- 1) In what ways can the module be credibly applied to evaluate nutrient sourceresponse relationships in the Delta under current conditions?
- 2) In what ways can the module be credibly applied to evaluate nutrient sourceresponse relationships in the Delta under modified hydrology, modified climate, modified Project operations and proposed conveyance facilities?
- 3) In what ways can the module be credibly applied to evaluate nutrient source-response relationships in the Delta under modified nutrient loading?
- 4) What would be other appropriate applications of the existing module?
- 5) What are the strengths and weaknesses of the recent module calibration and validation?
- 6) Is the module's conceptual formulation expected to lead to any systematic bias in nutrient concentration results?

# Findings

The need for numerical modeling of water quality processes in the Delta is clear, and well stated in the draft report:

"The recent decline in the health of the San Francisco-San Joaquin Delta (Delta) ecosystems has increased the importance of understanding ecosystem function, and the linkages between ecosystem health and system drivers such as water temperature and nutrient levels. *The complexity of these linkages presents a challenge that data analysis alone has not clarified, so conceptual and numerical models have been developed and used to increase our understanding of ecosystem functions.*" (emphasis added)

This statement identifies the critical need for a numerical model in the Delta to assess complex linkages between flow and physical, chemical, and biological conditions. Such linkages are necessary to assess conditions in the Delta and identify potential food web implications to address ecosystem attributes.

Review of modeling processes and representations in DSM2-QUAL documentation identified several pertinent points that would suggest a stronger basis for water quality modeling in the Delta than for other options such as data/statistical relationships. The use of DSM2 is a good platform to build from because of the generally accepted hydrodynamics and salinity (EC) applications in the past. However, implementing water quality modeling projects in large, complex systems such as the Delta can take a considerable amount of time. Not only are the stages of implementation and calibration resource intensive, the process of educating stakeholders and other involved entities and individuals regarding model representations and assumptions, data, and other supporting model information often occurs over a considerable time period.

The implementation of DSM2-QUAL as a Delta-wide water quality model (beyond salinity) is a sorely needed contribution to the water quality assessment "toolbox" for the Delta. The current DSM2-QUAL representation includes basic physical (temperature), chemical (nutrients) and biological (primary production) processes. The complexities of the Delta – hydrodynamics, meteorology, water quality, and operations – suggest the need for numerical models, but also present considerable challenges to modeling. Careful review of the model documentation and supporting information indicates that this effort is not intended to address all such water quality modeling challenges that could possibly exist in the Delta, but rather to lay critical groundwork through data review, model implementation, initial calibration, and preliminary application. As such, this project forms a valuable contribution.

Through several discussions with Marianne Guerin and/or Paul Hutton during the review process, considerable clarification on the project purpose became evident. One desired outcome of the development of a numerical water quality model of the Delta was to inform activities such as the current Bay Delta Conservation Planning processes. Apparently there are few available tools to address water quality concerns at the Delta scale, and a model would assist in such environmental review process.

Extending the existing DSM2-QUAL model applications to include basic water quality parameters is a logical and useful step. Through time, incremental improvements can be made in response to open and honest critical discussion, improved baseline data collection, completion of special or focused studies on specific processes, and acceptance of the model by the scientific and policy communities. An important aspect when participating in this evolutionary and developmental process is to avoid overly

constraining attempts to improve the available tools intended to advance the understanding of aquatic systems. Specifically, the science and policy communities' responsibility is to be both critical and supportive of such forward-thinking endeavors if progress is to be made in resolving complex issues such as those encountered in the Delta.

## **Response to Scope**

In response to the questions outlined in the scope, additional information is required. Specifically, the spatial and temporal elements of the questions being posed and the range of conditions hypothesized must be known.

Overall, the DSM2-QUAL application is the best available tool for assessing water quality in the Delta. This is not to say that it is perfect, a point which is clearly elucidated in the draft documentation and echoed in the various reviews. For example, the model is calibrated to monthly data. While application of the tool to short time scale problems is not recommended, the model can probably be applied as scoping or planning tool to assess monthly, seasonal trends, or annual trends. Because this is an initial application of a water quality model representing physical, chemical, and biological conditions, there are still elements of the model that require modification, improvement, and refinement.

In sum:

- Q: In what ways can the module be credibly applied to evaluate nutrient source-response relationships in the Delta under current conditions?
- A: Monthly, seasonal, or annual applications of the model will lend insight into system response and potential nutrient relationships. The complexities of the Delta extend beyond current model capabilities, so limitations exist. Still the model may be a useful tool for selected applications if employed responsibly and reasonably.
- Q: In what ways can the module be credibly applied to evaluate nutrient sourceresponse relationships in the Delta under modified hydrology, modified climate, modified Project operations and proposed conveyance facilities?
- A: the model has been tested under a wide range of conditions, but these conditions do not extend a highly modified hydrology, climate, project operations or proposed conveyance facility. If selected conditions vary considerably from historic data used in implementing the DSM2-QUAL model, uncertainty may increase markedly. The value of physically based models is the ability to extend them beyond historical conditions, but if the deviations are notably different, there is no guarantee that basing the model on conservation laws will ensure robust simulation results. Further, because the Delta is complex and data used to construct the current model are limited, care should be used (even when employing monthly or longer averages) in interpreting results. The model could be used as a gaming tool, to increase insight into potential system response, but this process should be considered as hypothetical exercise – an extension of a conceptual model.

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- Q: In what ways can the module be credibly applied to evaluate nutrient sourceresponse relationships in the Delta under modified nutrient loading?
- A: This answer is similar to the previous question. Using a model to extend one's knowledge of a system is an underappreciated use of these powerful tools (versus, for example, running limited "scenarios"). Even with considerable uncertainty in models, information can be gleaned from model application.
- Q: What would be other appropriate applications of the existing module?
- A: Planning level and scoping level analysis over long time periods, where order of magnitude estimates are appropriate. Insight to more detailed temporal or spatial questions, or to processes that are not incorporated into the model are more challenging. In certain cases the model can be used to gain insight into these more challenging issues, but care must be used in such assessments to ensure the results are meaningful.
- Q: What are the strengths and weaknesses of the recent module calibration and validation?
- A: Strengths include the long time series of information used in the simulations and the fact that temperature, nutrient transforms, primary production, and dissolved oxygen are all modeled in a physically based method (versus statistical relationships). Extensive data were assembled for the effort and the model was tested through various sensitivity analyses (both documented and undocumented). Several outstanding questions have been addressed (mass at the Martinez boundary). Weaknesses largely stem from the current formulation of DSM2-QUAL, data availability, and complexities in the Delta that are not well characterized in space or time. However, many of these weaknesses are recognized. Some are included directly in the documentation, while others are included in the comments to the draft documentation. Knowing model weaknesses is valuable knowledge. Models are imperfect tools, and knowledge of where inadequacies exist can allow even coarse models to be used to improve understanding and improve decision making.
- Q: Is the module's conceptual formulation expected to lead to any systematic bias in nutrient concentration results?
- A: Water quality models are useful because they encompass multiple, interrelated processes. In short, the critical fundamental processes should all be modeled as well as possible. The largest risk here is to focus on an element of the water quality model – like nutrients. Nutrients cannot be modeled properly if flow or temperature are not modeled well, or if primary production is not effectively represented, or if dissolved oxygen is not characterized properly. To assess the conceptual model formulation of DSM2-QUAL, a conceptual model of key processes in the Delta should be formulated – as a benchmark to "test" DSM2-QUAL and determine if the important processes are included in the current numerical model.

Model studies and analyses should be completing while considering limitations and uncertainty associated with the model. Further, in certain circumstances the model may simply not be able to represent the appropriate processes or to answer desired questions with sufficient confidence or resolution to be useful. Comments from this review and others should be, to the extent feasible, incorporated into the modeling work and documentation prior to further application. Certain comments and observations will require longer time periods, additional data, and appropriate funding to implement. As noted above, this is an initial foray into comprehensive water quality modeling in the Delta, but the effort hopefully will not end here.

### **Documents Reviewed**

The principal documentation was reviewed as were comments on the draft document. Two phone discussions occurred, one with Marianne Guerin and one with both Paul Hutton and Marianne Guerin.

Documents reviewed:

- Modeling the Fate and Transport of Ammonia Using DSM2-QUAL – Draft Final report (October 2009) and appendices

As part of this review, the comments that other entities had produced in response to the documentation were examined. Overall, considerable effort was expended by several reviewers of the report from a range of perspectives and disciplines. This information in itself is a worthwhile contribution to Delta water quality modeling. Comments were provided by:

- Larry Walker and Associates (via Sacramento Regional Wastewater Treatment Plant)
- Flow Science (via Sacramento Regional Wastewater Treatment Plant)
- Frances Brewster, Santa Clara Valley Water District
- Carol Kendell, U.S. Geological Survey
- Hari Rajbhandari, California Department of Water Resources
- Pat Gilbert, California Department of Water Resources
- Others (some comments did not have an author notes. Apologies to those unnamed individuals)

## **Comments on Comments**

Attempts have been made not to unnecessarily duplicate comments provided by other entities. In most cases other commentors have been careful to not only address an issue, but also to provide a solution or at least a direction for further exploration. Clarification of the objectives and approach, specifically the monthly time step approach to application would address a good fraction of these comments. Overall, considerable effort was expended by several reviewers of the report from a range of perspectives and disciplines. This information in itself is a worthwhile contribution to Delta water quality modeling. These comments illustrate that there is a great interest in the topic of Delta water quality, that there is considerable expertise available in aquatic system processes and modeling, and that the DSM2-QUAL is a platform that can be extended to fill an important need in the Delta.

# **Specific Report Comments**

#### **Executive Summary**

Several concepts key to the project could be more clearly presented in the executive summary. Two elements that are most prominent include:

- model resolution
- model calibration

Data limitations were clearly noted, but the decision to aggregate output to a monthly time step for calibration and application was not clear. Although the documentation states that calibration and validation statistics were calculated at a monthly time scale, the basis for that decision is not clearly stated. Further, the interesting aspect of calibrating for year types should also be noted. Detailed discussions later in the document provided more information, but adding several sentences in the executive summary would provide clarification about how this application proceeded and provide valuable information to the reader. For example, stating that considerable data limitations precluded calibration at a sub-monthly time step and that average monthly simulated values were used as comparisons to field data for calibration would clarify that the model is not, at the current time, intended to analyze sub-monthly (e.g., weekly, daily, or hourly) conditions. This addition would address several of the statements from some of the other reviewers of the draft documentation.

Other topics in the executive summary that merit comment include:

- Qualitative descriptions of calibration performance: terms like "very good," "good," "acceptable," are relative terms. Tying such terms to definable criteria can produce a more repeatable and quantitative result.
- Including the time step and spatial scale of the model would be useful for the reader. This would assist in identifying the implications of averaging simulation output to a monthly average for nutrients.
- Identification of additional monitoring needs is a valuable outcome of the project. Attempts to determine potential data needs without undertaking the process of model implementation would not have provided the critical insight necessary to fully identify data needs. Several commentors identified the need for additional data, mostly for time steps smaller than the monthly time period adopted in the project, and the executive summary clearly states that data need to be collected "at a time scale commensurate with the quality of desired results." There is additional work to be done to form a comprehensive water quality model of the Delta, but this is a valuable first step.
- The focus on nitrogen (and ammonia<sup>1</sup>) throughout the report detracts from the value of implementing a comprehensive water quality model in the Delta. Although an explicit objective was the assessment of nitrogen dynamics (or more specifically ammonia), to obtain this objective requires development of multiple elements of a water quality model because nutrient uptake interactions are

<sup>&</sup>lt;sup>1</sup> Ammonia will be using within this review, to be consistent the definition in the draft documentation.

temperature dependent and associated with phytoplankton production and mortality. Representing nitrogen and phosphorus, as well as phytoplankton processes is important.

- The identification of the need to define meteorological data on a regional basis is an important finding
- In general, doubling the length of the a executive summary would not be a burden on the reader, and would provide the author an opportunity to more comprehensively summarize key elements of the project and provide clear direction for those readers who wish to delve into the remainder of the report.

#### 2. Project Objective

Principal objectives identified in the documentation include:

- 1. Calibrate and validate DSM2-QUAL to simulate temperature interactions, with a focus on ammonia and nitrogen dynamics, in the model domain from 1990-2008.
- 2. Develop a prioritized water quality monitoring programs with the intent of improving understanding of ammonia and temperature dynamics within the Delta and improving the quality of model calibration.
- 3. A separate objective is to critique and provide potential modifications to the current conceptual model used in QUAL to simulate nutrient dynamics in the Delta.

Comments:

- Recommend that the objective of potential model applications be introduced in this section. Specifically, state what the expected or intended use or uses of the model are. Examples may include planning and scoping level studies where comparative analysis would be applied.
- Identifying that conceptual models have been developed to define potential linkages is useful. Please clarify what is meant by conceptual models. For example do these conceptual models identify potential spatial and temporal scales? If so, was the DSM2-QUAL application consistent with the temporal scales identified as important? If not, how might the DSM2-QUAL model further inform a broad conceptual model formulation of water quality throughout the Delta in space and time? See additional comment under §5.

#### § 3. Background

- Some background on water quality in the Delta would be useful to set the stage for the potential realm of applications for this tool. That is, what kinds of questions are being asked at the current time, what are the working hypotheses? This would provide a foundation for the current modeling to stand upon a reason to complete this work because there is a clear need. This can also tie into the monthly time step for calibration and application.
- An expanded section on previous Delta water quality modeling would be a useful addition and illustrate that this current work is a contribution. Including a review of previous modeling efforts, including statistical or empirical models, analytical models, and numerical models would elucidate the need for such water quality models.

- \$3.2 would be more valuable to the reader with a broader description of the problem, processes involved, and role in the Delta.

#### §4. Model Configuration

- The model grid is presented graphically in the appendix. Additional information about the construction of the grid from a spatial representation perspective would inform the reader why there are areas of high resolution and areas of low resolution. This spatial resolution could also be coupled with selection of model time step information. This latter point would assist in explaining the use of monthly data and averaging simulation results up to the monthly time step (which is not the same as the simulation time step of DSM2-QUAL) for model calibration and application.
- Under model boundaries (§4.2), uncertainty in estimated parameters is identified as a potential limitation: "The uncertainty in the estimates of DICU inflow, outflow and concentrations is high. During periods of low inflow, errors in volumes ascribed to DICU boundaries may dominate model results." This type of information is invaluable, and the fact that this topic is picked up in §16 (Next Steps) as a data need is good. Recommend adding this topic to monitoring needs in §14.
- Under §4.2.2 there is note that salinity is not important in nutrient dynamics of the model. From a primary production standpoint, changes in salinity can affect algal species composition and standing crop. Changes in these algal community conditions could have an affect on nutrient uptake. This may be a minor point.
- Identifying that a single meteorological region is insufficient for temperature modeling in the Delta is a valuable finding. Suggest adding recommendations for necessary spatial and temporal coverage in the monitoring section and next steps (§14 and §16)

#### §5. Conceptual Model for Nutrient Dynamics

- §5.1 please clarify for the reader the assumption of representing the constituents as non-conservative versus conservative.
- Although a conceptual model is presented in the draft report as a process diagram for DSM2-QUAL, this figure does not represent the actual conceptualization of key processes in the Delta. Without a clear picture of key physical, chemical, and biological processes in the Delta, there is no benchmark to compare the current DSM2-QUAL formulation. Therefore, there is no real mechanism to determine if DSM2-QUAL is representing critical processes and linkages. Discussions with the report author identify that much of this information was included in a previous draft. Recommend that some of this material be incorporated into the final draft, summarizing what processes are represented in DSM2-QUAL and what processes are not...and if those not present are potentially important. Those processes that have modest or minimal implications in the Delta can be placed at a lower priority. This framework provides a "bookkeeping" system that ensures, to both the analysts and the stakeholders that the broader range of issues has been considered, and those with the higher priority can be incorporated into the modeling process. Further, such a system provides a mechanism to revisit

existing processes or incorporate new processes as additional information and data become available. As such, conceptual model documents are often referred to as "living" documents.

- The equations representing the dynamics of the various constituents are useful, particularly to one familiar with representing such processes in a model. Recommend identifying all variables in these equations as you proceed through the discussion so the reader can readily identify the discrete processes within each equation.
- Presenting all model parameters in tabular form presents an easily readable summary. Recommendations and comments on Table 5.2 include:
  - Through conversations with the author, the range in parameter values for certain parameters (e.g., organic nitrogen settling rate, organic phosphorus decay rate, organic phosphorus settling rate, etc.) is due to retaining parameter values from past DSM2-QUAL applications in the south Delta and calibrating new areas of coverage separately. Recommend identifying why and where the ranges of for certain calibrated values apply in the spatial domain. If values vary temporally, which is not expected, detailed discussions describing such variations are needed.
  - Organic matter in DSM2-QUAL is partitioned into organic N and organic
    P. Should settling rates for these two constituents should be similar?
  - Nitrite decay rate at  $2 \text{ day}^{-1}$  is about twice literature values.
  - Is benthic release rate for orthophosphate a function of low dissolved oxygen concentrations in DSM2-QUAL? At what dissolved oxygen level does orthophosphate release rates become appreciable? If this is simply loss from the bed by another process, please identify.
  - For many rates, Table 5-2 identifies that the rate coefficients are "at ambient temperature." However, these rates are typically represented in literature at 20°C, and are corrected to ambient temperatures through the temperature coefficients listed in at the bottom of Table 5-2 (e.g., via an Arrhenius or van't Hoff relationship).
  - Benthic oxygen demand rates seem extreme. Recommend checking units because 30 to 200 g m<sup>-2</sup> d<sup>-1</sup> is one to two orders of magnitude higher than typically observed values in eutrophic systems. The Chapra (1997) rates are typical values. Perhaps units are mg m<sup>-2</sup> d<sup>-1</sup>.
  - There is discussion in §3.2 about ammonia interfering with phytoplankton growth. In DSM2-QUAL there is an ammonia preference factor. These two items appear to be contradictory. There is a rich literature on ammonia preference that continues to be updated. Recommend exploring a range of literature on both ammonia interfering with phytoplankton growth and ammonia preference.
  - Some units in the table are in English, others in SI
  - Half saturation constants for nitrogen look a little low, while one could argue that phosphorus half saturation constants may be a little high. The magnitudes are less important than the testing of sensitivity around these two parameters, which can have profound impacts on inorganic nutrient and phytoplankton dynamics in aquatic systems.

- The ratio of chlor\_a to algal biomass is typically unitless (i.e., in equivalent units in the numerator and denominator (e.g., ug Chlor\_a/ug of Algae). DSM2-QUAL water quality logic is derived from QUAL2E (Brown and Barnwell, 1987<sup>2</sup>). Review of the QUAL2E manual identifies units of ug Chlor\_a/mg of Algae, i.e., mixed units. A review of the QUAL2E code would be required to determine if the conversion of micrograms to milligrams is done internally, or if this is a typographical error. If this logic were directly transferred to DSM2-QUAL, this ratio and units should be investigated.
- Should settling rates for organic N, organic P, and CBOD be in units of [Length/Time]? They are not shown this way in the governing equations (like algae settling).
- Units on phytoplankton mortality rate are in ft day<sup>-1</sup>. Typical units would be day<sup>-1</sup>. Further, 0.7 day<sup>-1</sup> mortality rate would be higher than typical literature values, depending on how mortality is defined. Occasionally, models will combine respiration, mortality, and grazing, which can lead to values close to this number. DSM2-QUAL appears to separate out respiration and grazing is explicitly not included. Recommend clarifying assumptions regarding selected values.

#### § 6. Data Sources and Data Refinement

- §6.2:
  - Please clarify what is meant by "measurement methodology." Were laboratory methods and collection methods reviewed (e.g., were quality assurance project plans or field sampling standard operating procedures reviewed)?
  - Recommend reminding the reader that the intended temporal resolution of the model is monthly, although model simulations occur at 15 minute time steps.
  - Are there limitations of using linear interpolation on irregular time series with regards to model calibration assessment?
- §6.3:
  - Qualitative terms such as "good," "poor," or "not very good" are common in this section. Recommend developing, at a minimum, a consistent set of adjectives. If a quantitative measure could be developed, such as data collected under
    - a USGS protocols,
    - a detailed quality assurance project plan,
    - data came with quantifiable accuracy (e.g., remote logging thermistors)
    - etc.

it would be easier to rate the data. This may not have been feasible under resource (time, money) constraints. This could be included in §14 and §16 if such an approach is deemed useful for future modeling.

<sup>&</sup>lt;sup>2</sup> Brown, L.C., and T.O. Barnwell. 1987. The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and User Manual. EPA/600/3-87/007. May.

- Perhaps insight into organic phosphorus concentrations can be gleaned from existing data. Organic phosphate calculated as total phosphorous (TP) minus orthophosphate may be appropriate under certain circumstances (if sufficient information is known about the sample processing). If orthophosphate is reported as soluble reactive phosphorus (SRP), then the difference of TP minus SRP can be (a) dissolved and particulate organic P, or (b) dissolved and particulate organic P, plus orthophosphate adsorbed to clay particles. If non-volatile suspended solids concentration is low, TP minus SRP may be acceptable. If the converse is true, then a notable portion of orthophosphate could be adsorbed to nonvolatile suspended solids. Perhaps information from the monitoring plans (or as recommendations for future monitoring plans) can be reviewed to lend insight into non-volatile suspended solids concentrations. In either case, review of TP – orthophosphate data would lend insight into the potential range of organic P values present in the Delta and constrain the range of values used on formulating organic P concentrations employed in the DSM2-QUAL Delta application. Recommend including a discussion in the documentation more formally identify the challenges around estimating organic P in DSM2-QUAL, which could lead to recommendations in §14 or §16.
- §6.4:
  - Documentation on missing data is generally omitted from model reports or dismissed with a sentence or two. Although not exhaustive, outlining approaches and assumptions is a valuable section included in the model documentation. Coupled with the information in the Appendices, this information indicates that considerable thought and effort were undertaken to utilize the available data to the highest degree.
  - In the last paragraph censored data are discussed in light of model 0 uncertainty, which raises the question: what is the accuracy of this DSM2-QUAL application? In §10 there is extensive discussion concerning the goodness of fit, but quantitative measures are not presented therein. In the appendices there are quantitative goodness of fit measures (e.g., bias, mean squared error, root mean squared error, etc.) for temperature simulations. Recommend pulling some of this valuable quantitative information up to the main document to illustrate accuracy and uncertainty of the model at various calibration and validation locations within the Delta. Selected graphical information could be used to illustrate that the model tracks seasonal variations and short term variations. Consider similar quantitative discussion of nutrient performance versus "very good," "good," "satisfactory," and "unsatisfactory," and sending the reader to the appendix for a table of rating definitions for multiple statistics that may not be readily interpreted in terms of model uncertainty. If the presented statistics are deemed the best for the job, perhaps add additional discussion so, for example, a decision maker could more easily interpret the amount of uncertainty in model results for each constituent.

• Graphical comparison of different data sets was an effective way to illustrate variability between multiple data sets, data resolution, and challenges of interpolation. Very informative.

#### § 7. Data Availability: Time Span and Locations

- The authors do an admirable job of laying out data availability. This is a tough job, but the work here is clearly a needed contribution. Models can always benefit from more data, and this is a good effort to assemble available information. One of the most valuable attributes of applying a numerical model such as DSM2-QUAL is that the exercise requires quantifying many attributes of the system that in itself is a constructive process.
- §7.7.3 Minor point: DO is not generally considered a nutrient.

#### § 8. Setting Boundary Conditions

- The exploration of loss of mass at Martinez is very useful.
- \_ General comment: in several sections boundary conditions are modified, adjusted, etc. In some sense this is part of the "art" of modeling. The documentation on these points is uneven. This is mostly an organizational element to aid the reader - if the boundary condition locations were presented in same order for each constituent and given the same level of discussion (where appropriate) was provided on adjustments and assumed concentrations the document would be more robust. For example, ammonia at the Sacramento River boundary condition was modified by a factor and model performance was assessed while developing this boundary conditions. This is a useful discussion. For other locations, where no data were available, such as the Yolo or Lisbon Toe Drain boundaries, values were set at 0.03 and 0.04 mg/l, respectively. There is no discussion of what these values are based upon. These are reasonable values for ammonia concentration, and a simple sentence or two that states these would be typical values for ammonia in aquatic systems where organic nitrogen is low or modest and oxygen concentrations are near saturation...or maybe this is not the case for Yolo or Lisbon Toe Drains. Reading these sections where numbers are simply stated as assumed concentrations with no background or basis leaves the reader wondering where they came from.
- §8.2 Meteorology: several "factors" are used to adjust wind speed spatially and temporally. This suggests a need not only for regionalized meteorological representation, but also associated meteorological monitoring.
- §8.3 How were the constant values for boundary conditions temperatures set at 9°C determined?
- §8.4 Organic N and organic P values should be related, approximately, by stoichiometry if they share a principal source (allochthonous or autochthonous). However, organic P boundary conditions at the Yolo or Lisbon Toe Drain are 1/20<sup>th</sup> that of organic N.
- §8.5 Recommend setting DO boundary conditions based on saturation (function of temperature and elevation) versus constant values for Mokelumne, Cosumnes, and Calaveras Rivers, although these small sources probably do not affect simulations appreciably.

#### § 9. Chemical Speciation Modeling and Isotope Analysis

- This topic should be included as a sub-section in section 14 or 16 as future studies or research. For a model used at a monthly time scale this is not an issue. The Delta may have a few areas where conditions exist to experience persistent, elevated pH (e.g., 9.0 for more than a day or two), but assessment of such conditions would require a model with considerable local detail (and associated data to drive it) and a much finer time scale (sub-daily) to analyze with certainty these conditions. Adding pH to DSM2-QUAL is a laudable goal and the reviewer does not want to discourage such modifications, but such modifications should be consistent with the realm of modeling applications (which is currently monthly).

#### § 10. Calibration and Validation

- For this application the calibration of temperature independent of water quality is acceptable.
- The ability to apply the model over extended time periods is helpful. This allows the model to be assessed over various hydrologic year types, variable meteorological conditions, and for different water quality circumstances. The extended simulation time period also allows the analysis to take advantage of the variably available data, which was not consistent through the 1990-2008 period.
- For temperature calibration, the documentation identifies that the previous calibration (Rajbhandari 2003) was applied to the south Delta and the remainder was calibrated under the current effort. If this is the case for the water quality component, please note as such.
- The process of calibrating and validating to year types and spatial areas should be described in greater detail. The calibration methodology sections are quite short less than a page. The pros and cons associated with spatially available data could be discussed in light of the objective or intended application. There is appreciable information in the document. The Delta is a large area and the simulation extends for nearly two decades. Summarizing all of the calibration results is not an easy task. However, over simplifying by averaging over space or time can often mask underlying model performance issues. The regionalization may help in this case, and the hydrologic year-type information may help as well. However, water quality processes may not, particularly at critical periods of the year (e.g., summer), respond strongly the hydrologic year type. Are the regions identified herein recommended for future modeling studies as well? Could refinement be made, and if so, what, how, where, and when? Any recommendations could be incorporated into §14 and §16.
- Twenty regions for setting unique water quality parameters seems excessive depending on the parameters chosen. Please clarify where the listed parameters were changed and supporting assumptions or information. Table 5.3 does not provide sufficient detail on this point. Recommend minimizing changes among regions for parameters that would tend to be more globally uniform. For example, the process of hydrolysis of organic N to NH3 probably does not change between locations in the Delta. Decay rates for ammonia, nitrite and organic P also are probably stable. If they are not, and there is good reason to vary them,

then documenting assumptions will suffice. Without such documentation the modeling calibration may be interpreted as "curve fitting" exercise and can diminish the robustness of the calibration.

- Did the two year types for water quality calibration (wet and dry) provide any additional information than simply calibrating with all the years? This holds for temperature too (where four year types were employed). What was the impetus for year type calibration?
- § 10.3.1 For algae related parameters, a fair amount of discussion was presented, with several literature sources cited. Recommend identifying clearly the ultimate selected values (or referring the reader back to Table 5.3). Also, is the Delta P-limited, N-limited (might this change with time of year or spatially), or is this known?
- The reviewer appreciated the data challenges facing the author regarding calibration and validation. A few notes.
  - The PBIAS criterion is insensitive, yielding "very good" calibration almost 90 percent of the time.
  - The scale for rating calibration performance is unsatisfactory, satisfactory, good, and very good. Of these four categories, three of them are satisfactory or better. Does this affect the calibration assessment?
  - Recommend bring Figures 17-15 through 17-17 into the main body of the report. These figures show the full range of performance metrics over the calibration/validation period and would provide the reader with a quantitative presentation and support the qualitative criterion in Figures 10-1 through 10-3.
- §10.4 Identification that the calibration parameter set is non-unique is important. However, even with parameter values within the ranges identified in literature and "reasonable" estimates at system boundaries, uncertainty is not well quantified in complex systems such as the Delta which exhibit non-linear responses to physical, chemical, and biological processes. Certainly time, resources, and data constraints limited the exploration of even a partial range of potential outcomes. Thus, as an initial foray into the Delta, the implementation and calibration exercises are clear contributions, in what will hopefully be a long term process of improving numerical modeling in the Delta. Recommend reinforcing with the reader that the model is currently calibrated to monthly data and as such is most applicable to monthly to seasonally or longer time horizon applications.

#### § 11. Volumetric Fingerprinting and Liberty Island Grid

- These are very interesting applications of the models. The fingerprinting analysis lends insight into contributions and the Liberty Island modification is a useful sensitivity analysis. What is the conclusion from the fingerprinting analysis? If nothing else it is a useful tool when interpreting results. Might add the need for monitoring in the vicinity of Liberty Island to §14.

#### § 12. Scenarios – Sensitivity to Changes in N-Concentrations

- Recommend providing a lead in paragraph explaining the purpose of the scenarios, as well as the choice of particular scenarios.

- A sensitivity assessment of a wider range of parameters (beyond nitrogen forms) would also provide a broader examination of model performance, e.g., a good way to test assumptions about organic P representations (or lack thereof). Focusing on nitrogen without phosphorus, or algae limits the efficacy of the simulations.
- Clarify the calculation of the "average monthly percent change" for the tabulated results. Are there years or periods within a year that might be of more or less interest?
- \$12.9 Attempting to model clams in the current DSM2-QUAL framework was probably overreaching a point acknowledged in there report. An interesting experiment and probably a good learning experience.

#### § 13. Model Enhancements

Key points identified herein regarding model enhancements include:

- a need for spatial meteorological representation for temperature simulation
- the value of multiple algal groups
- potential role of bacteria
- macrophytes or submerged aquatic vegetation
- benthic interactions
- mass balance
- organic matter (variable CBOD demands)
- pH

Some general comments on these topics are:

- <u>spatial meteorological representation</u>: this is a valuable addition
- <u>multiple algae groups</u>: Multiple algal groups, as noted in the document, would be valuable, particularly with the current interest in cyanobacteria blooms in regions of the Delta
- <u>bacteria</u>: this is a challenge to model, and modeling multiple species can add to the burden
- <u>macrophytes et al</u>: these can be challenging to model due to the wide range in form of different species, as well as the various forms a species may undertake in response to different environmental conditions. However, for regions where widespread macrophyte growth occurs or is important, such conditions could potentially be quantified and modeled.
- <u>benthic interactions</u>:
  - <u>clams</u>: clams or similar benthic fauna would require collection of species specific information regarding the potential implications on water quality and the sediments. Spatial and temporal distributions would be required, as would life stage specific information.
  - <u>bacteria</u>: modeling biofilms and bacteria on a large scale is limited at current time to research activities.
- <u>mass balance</u>: moving from CBOD to organic matter (see below) and a more comprehensive sediment compartment representation, and tracking of mass loss to/from the bed (for example) can reduce some of these issues. Full sediment digenesis is desirable, but may be cumbersome. (The mass balance issue at the downstream boundary is also a point of interest.)

- <u>organic matter</u>: a more representative treatment of organic matter and explicit representation of organic matter fractions (i.e., carbon). For example, the refractory, labile, particulate, and dissolved representations in CE-QUAL-W2 would improve representation of carbon, nitrogen and phosphorus, settling of organic matter (and DO and SOD). This would require a move away from modeling CBOD as a state variable.
- <u>pH</u>: pH can readily be added to the model, but would recommend a more comprehensive assessment for need and purpose.

Associated with these additions would be increased data needs (e.g., increase the need for monitoring), which can be a resource and funding challenge. However, model updates are relatively straightforward and much of the model logic structure is probably in place to handle input/output changes and additional state variables, i.e., this would not require a re-write of the entire model...but the model would certainly be more comprehensive.

Other comments:

- Several production models exist that are much more comprehensive than the current DSM2-QUAL (QUAL2K, CE-QUAL-W2, WASP). This increased complexity can increase uncertainty, but the flexibility of having the option to explore processes and interactions in more detail generally outweighs the additional complexity. In this first application of DSM2-QUAL to the Delta, the approach has been appropriate and useful. Through time, and in response to increased understanding, a logical path may be to incrementally add detail to the existing model.

#### § 14. Monitoring Program

- The monitoring program section is a useful and pertinent section of the report.
- Three elements of monitoring were identified: temporal (i.e., frequency), spatial, and cost. Cost was not explicitly considered, but raising this vital point is valuable.
- The report identifies that the quality of data was better in more recent years (2000 to present) but spatial coverage was better historically (1990-95). The term "better" is vague. In several instances there are references that state "sufficient" data was available to complete the desired modeling. Tying modeling objectives to required data needs will help explain what level of data are required and provide a ready metric for defining what is "sufficient" and what is meant by "better." Recommend a more rigorous monitoring assessment, clearly defining specific locations, frequencies, and parameters (versus "regions"). If this was beyond the scope of work, it may be useful to identify this as a resource limitation and perhaps include a formal recommendation to develop a monitoring program designed to support water quality modeling.

#### **§15. Summary and Conclusions**

- Recommend identifying that the model was calibrated at a monthly time step and is useful for monthly or seasonal predictions. Further, identifying that a long

simulation period (variable hydrology, meteorology, and water quality) is a strength – a point that has not been presented clearly in the document.

#### §16. Next Steps

- Recommend updating the "Next Steps" and adding a recommended priority for each item (e.g., high, medium, or low) to the various items to guide policy makers.
- If the model cannot effectively take into account Corbula, then extending the model back to "pre-Corbula" periods may not be a high priority.

#### §17. Appendix I

- Appendices 17.1 through 17.10 are a notable contribution to water quality modeling in the Delta. Clearly a considerable amount of work went into gathering and documenting a significant amount of data and information. Also, presentation of boundary conditions data (including in tabular and graphical presentations) is a useful and good practice in model documentation. Following this up is valuable documentation of boundary conditions of these methods. Including methods for calculating model parameters (e.g., wet bulb, ammonium ionammonia) is helpful to readers as well. Laying out calibration performance metrics in fact multiple metrics in §17.9 further reflects good documentation practices. Such information also provides a clear roadmap for current and future modeling efforts to build upon.
- Appendix 17.9.2 Recommend not sending the reader to a citation for discussion of why only selected statistics were employed for nutrient results assessment. Simply explain the logic in the citation and how or why it applies to the DSM2-QUAL Delta application. Several other statistics are included in the tables, and probably provide insight into model performance. Is there a reason these were not included in interpretation? Finally, recommend a discussion describing the methodology of aggregating model output to monthly average to compare against monthly field data. An important assumption in this method is that the nutrient grab sample is assumed to represent a monthly average to be compared with a monthly average based on simulated concentration. However, there may be considerable limitations in assuming the grab sample is representative of monthly conditions. For certain constituents, at certain locations, at certain times, this approach may be satisfactory.

The topic of monthly averaging results and model temporal resolution brings up a general, but simple modeling rule of thumb regarding time step and model output interpretation. Model performance typically improves when averaged to a longer time period. For example, model performance metrics of an hourly calibrated model is typically better when averaged to daily values. Similarly for daily models averaged to weekly values, weekly model averaged to monthly values, and monthly models averaged to seasonal values. For the DSM2-QUAL model, which is calibrated at a monthly time step, the logical interpretation would be seasonal periods, particularly because averaged monthly data were compared to monthly grab samples. The fact that monthly data are used is clearly documented, and thus the model was not intended to be used to assess hourly, tidal cycle, diel system response, or even weekly responses. Rather, an appropriate application would be for monthly or several month interpretations. The 19 year simulation period provides a long time period, including multiple hydrologic year types, which allow monthly or seasonal interpretations to potentially provide considerable value. Simulation results (presented monthly) clearly indicate intra-and inter-annual variations and can lend potential insight into variable boundary influences on conditions within the domain.

- Appendix 17.12 – estimating mass loss at the Martinez boundary in DSM2 – is a good exercise. This particular issue has haunted Delta modelers for decades, and rather than neglect the topic it is clear that a considerable amount of effort was put forth to quantify loss of mass under various conditions (flow ranges and tidal excursions). This appears to be the first effort to quantify in a systematic fashion this process. If the author has recommendations or ideas on how to further accommodate boundary conditions in Delta DSM2-QUAL applications, these would be welcome additions to the report.