Modeling hypoxia in the Chesapeake Bay: Ensemble estimation using a Bayesian hierarchical model

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ABSTRACT

Quantifying parameter and prediction uncertainty in a rigorous framework can be an important component of model skill assessment. Generally, models with lower uncertainty will be more useful for prediction and inference than models with higher uncertainty. Ensemble estimation, an idea with deep roots in the Bayesian literature, can be useful to reduce model uncertainty. It is based on the idea that simultaneously estimating common or similar parameters among models can result in more precise estimates. We demonstrate this approach using the Streeter–Phelps dissolved oxygen sag model fit to 29 years of data from Chesapeake Bay. Chesapeake Bay has a long history of bottom water hypoxia and several models are being used to assist management decision-making in this system. The Bayesian framework is particularly useful in a decision context because it can combine both expert-judgment and rigorous parameter estimation to yield model forecasts and a probabilistic estimate of the forecast uncertainty.

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1. Introduction

Bottom-water hypoxia (dissolved oxygen ≤2 mg l^{-1}) has become common in many coastal marine ecosystems (Diaz, 2001), causing stresses in some estuarine species (Eby et al., 2005; Craig and Crowder, 2005). Hypoxia is generally attributed to eutrophication induced by excessive nutrients, though other sources may contribute to oxygen demand (Mallin et al., 2006). Low oxygen conditions were first reported in Chesapeake Bay in the 1930s (Newcombe and Horne, 1938; Officer et al., 1984). Though hypoxia may have been an intermittent natural phenomenon, sediment core analyses indicate that the frequency and extent of Chesapeake Bay hypoxia increased with European settlement in the watershed and the consequent land cover changes (Cooper and Brush 1991; Cooper 1995).

Reducing the severity of Chesapeake Bay hypoxia is an important restoration goal, and several water quality models have been used to help decision-makers estimate the pollutant load decreases needed to attain the desired improvements. The complexity of these models has ranged from a three-dimensional dynamic model (Cerco and Cole, 1993) to simpler statistical relationships (Hagy et al., 2004). The range of modeling approaches used in Chesapeake Bay reflects an ongoing debate among water quality modelers regarding the relative utility of complex vs. simple models (Borsuk et al., 2001), each with characteristic advantages and disadvantages. If we understand the important system processes and can express them mathematically, then process-based models should provide reliable predictions of system behavior. Alternatively, statistical models help quantify predictive uncertainty; however, statistical models rarely have an explicit mechanistic basis, reducing their confidence for use in predictions outside the bounds of past observation.

More recently, Scavia et al. (2006) used a compromise approach, applying the Streeter–Phelps equation (Streeter and Phelps, 1925), a simple process-based model to describe Chesapeake Bay dissolved oxygen (DO) patterns. The Streeter–Phelps dissolved oxygen model can be written as:

$$DO = DO_s - \frac{k_1 BOD_u}{k_2 - k_1}\left(e^{-k_1 \frac{x}{v}} - e^{-k_2 \frac{x}{v}}\right) - D_i e^{-k_2 \frac{x}{v}} \qquad (1)$$

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where DO=the dissolved oxygen concentration (mg/L), DO_s= the saturation oxygen concentration, k_1=the BOD decay coefficient (1/day), k_2=the reaeration coefficient (1/day), BOD_u=the ultimate BOD (mg/L), x=the downstream distance (km), v=stream velocity (km/day), and D_i=the intitial DO deficit (mg/L). This model describes the DO depletion that occurs when oxygen consuming substances initially remove oxygen from a stream and subsequent recovery as reaeration occurs. This approach to modeling coastal and estuarine hypoxia has also been used successfully for the Gulf of Mexico major hypoxic region (Scavia et al., 2003, 2004).

Herein, we extend the approach of Scavia et al. (2006) and implement a Bayesian version of the Streeter–Phelps Chesapeake Bay model, exploiting available dissolved oxygen measurements to estimate model parameters and inputs of interest, and their uncertainty. The Bayesian approach provides a rigorous framework for uncertainty analysis (Pappenberger and Beven, 2006), a useful component of model skill assessment, which also yields key information for management decision-making (Reckhow, 1994). Bayesian inference is based on Bayes Theorem:

$$\pi(\theta|y) = \frac{\pi(\theta)f(y|\theta)}{\int_\theta \pi(\theta)f(y|\theta)d\theta} \qquad (2)$$

where $\pi(\theta|y)$ is the posterior probability of θ (the probability of the model parameter or input vector, θ, after observing the data, y), $\pi(\theta)$ is the prior probability of θ, (the probability of θ before observing y), and $f(y|\theta)$ is the likelihood function, which incorporates the statistical relationships as well as the mechanistic or process relationships among the predictor and response variables. In many modeling applications $\pi(\theta)$ is a set of fixed values (probability distributions with a probability mass of one on a particular value for each θ), often based on precedent, experience, or tabulated literature values (Bowie et al., 1985).

Scavia et al. (2006) used fixed *a priori* values for the model parameters based on a combination of available information and expert judgment. While Scavia et al. (2004, 2006) used Monte Carlo analysis to characterize prediction variance due to uncertainty in one of the model parameters, v, Bayes theorem provides a rigorous framework to simultaneously relax more of the fixed model inputs and incorporate uncertainty in these values by expressing them as probability distributions. Higher uncertainty is expressed by choosing a large variance for the prior distribution, while more certain values can be represented with a smaller prior variance (with a fixed point value being the extreme case of absolute certainty). If there is little prior information available about a particular input value, then a non-informative (also called vague or diffuse) prior distribution can be used. A non-informative prior generally has a very large variance and minimally influences the posterior distribution of θ. The posterior distribution, $\pi(\theta|y)$, is a weighted combination of the information conveyed by the prior distribution and the likelihood function (i.e. the combined model and data). Thus, if the data contain a lot of information about the value of θ (as conveyed via the likelihood function) even a prior distribution with a small variance may have only a modest influence on the posterior distribution.

Using Bayes theorem there is no distinction between model parameters and other unknown model inputs such as unobserved initial conditions, missing values of state variables, or external inputs. Any unknown quantity can be estimated if the combination of the prior distribution and likelihood function provide sufficient information. In the Streeter–Phelps equation k_1, k_2, and v would typically be considered the model parameters, which could be estimated from data, while DO_s, DO_i, and BOD_u are measured boundary conditions, initiation conditions, and observed inputs, respectively. However, with sufficient data for DO and x, any of these parameters and/or inputs can be estimated and, in fact, the mathematical structure of the Streeter–Phelps equation makes it possible to estimate all of them simultaneously, although extreme correlation can impose numerical difficulties when estimating some parameter/input combinations.

An important difference between Bayesian methods and most parameter estimation approaches is that Bayesian inference emphasizes using the entire posterior distribution of parameter values, not just a single set of optimal values. This feature can be particularly important when the posterior distribution is asymmetric with optimal values that are different from the mean values (Stow et al., 2006), or when the model response surface is nonlinear. Predictions for unobserved or future ys (denoted $\tilde{y}$) are assessed over the entire posterior parameter distribution as:

$$\pi\left(\tilde{y}|y,\theta\right) = \int_\theta f(\tilde{y}|\theta)\pi(\theta|y)d\theta \qquad (3)$$

which is referred to as the predictive distribution. Eq. (4) indicates that, future y values are predicted by considering all probable combinations of the parameter vector θ, which translates into a mapping of the distribution of θ to a distribution of $\tilde{y}$. The predictive distribution incorporates prediction uncertainty resulting from uncertainty in all estimated model inputs, including their covariance, as well as the model error term and uncertainty in the model error variance.

2. Methods

Scavia et al. (2006) used the Streeter–Phelps model to calculate summer steady-state sub-pycnocline oxygen concentration profiles along the main stem of the Chesapeake Bay (Fig. 1) for each year from 1950–2003. Because the Chesapeake Bay is vertically stratified with surface waters flowing seaward and bottom waters flowing landward, they estimated sub-pycnocline oxygen demand as a point source of organic matter, proportional to Susquehanna River nitrogen load, at the southern end of the mid-Bay region (ca. 220 km from the Susquehanna River mouth). While physical and biological processes relating external nitrogen loading to hypoxia are actually quite complex, the model's ability to reproduce the observed interannual variability in both profiles and hypoxic volume, and the fact that the model calculates a theoretical profile at steady state (as opposed to via detailed temporal dynamics), help justify their use of the simplifying assumptions.

DO profiles of data were computed from interpolated observations that populated a regular grid with dimensions, first at 1-m resolution in the vertical and then at 1-km in the horizontal across constant depths (Hagy et al., 2004). From this grid, we produced down-estuary profiles for 137 values

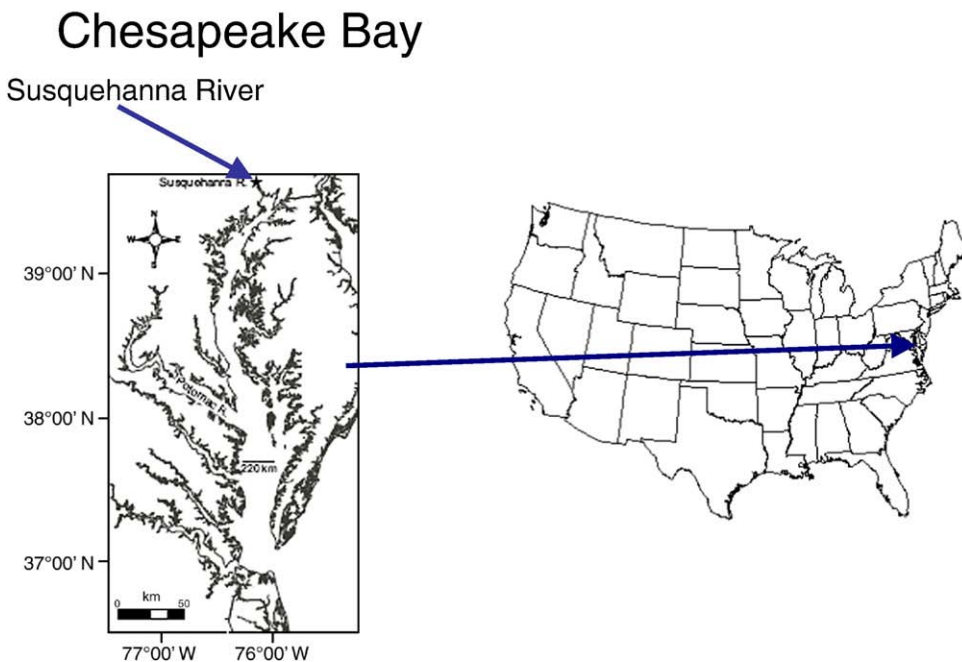# Chesapeake Bay

Susquehanna River

Fig. 1. Location map of Chesapeake Bay

along the ~220 km transect for each of the 36 years from 1950–2003 that we used in our analysis.

Historically, the practical implementation of Bayesian methods was limited because most non-linear process-based models result in mathematical forms that are analytically intractable when incorporated into Bayes theorem. Thus, numerical estimation was required which made applications using models of more than a few dimensions impractical because of the extensive computer time needed. However, the advent of fast, cheap, and widely available desktop computing has fostered development of algorithms that make numerical estimation for Bayesian approaches feasible (Gelfand and Smith, 1990). These Markov Chain Monte Carlo (MCMC) algorithms begin with user-provided start values and after a sufficient "burn in" period converge in distribution to the posterior. Once converged, they effectively provide a representative, proportional, random sample from the posterior distribution. The resultant sample can then be used to precisely estimate any function of the posterior distribution by plugging the sampled values into the function. To implement our model, we used WinBUGS, a free, downloadable MCMC software designed for Bayesian applications (Gilks et al., 1994). All of our inference is based on samples of 1000 taken from the posterior distribution after a sufficient "burn-in" to ensure the MCMC algorithm had converged.

To incorporate the Streeter–Phelps model (Eq. (1)) into Bayes theorem (Eq. (2)), we added an error term, ε, to the model and assumed ε to be normally distributed with zero mean and variance of σ^2. This assumption is consistent with nonlinear regression methods based on least-squares or maximum-likelihood optimization approaches (Bates and Watts, 1988). Additionally, Scavia et al. (2006) incorporated a term, F, to estimate the fraction of surface organic carbon

production that settles below the pycnocline. With the inclusion of an additive error term, ε, Eq. (1) becomes:

$$DO = DO_s - \frac{k_1 \times F \times BOD_u}{k_2 - k_1} \left(e^{-k_1 \frac{x}{v}} - e^{-k_2 \frac{x}{v}} \right) - D_i e^{-k_2 \frac{x}{v}} + \varepsilon. \quad (4)$$

If ε is assumed to be independent and normally distributed with mean=0, and variance=σ^2 then Eq. (4) is incorporated into the following likelihood function:

$$\prod_{h=1}^{137} \frac{1}{\sqrt{2\pi\sigma^2}} exp \left[\frac{\left(DO_h - DO_s + \frac{k_1 \times F \times BOD_u}{k_2 - k_1} \left(e^{-k_1 \frac{x_h}{v}} - e^{-k_2 \frac{x_h}{v}} \right) + D_i e^{-k_2 \frac{x_h}{v}} \right)^2}{-2\sigma^2} \right] \quad (5)$$

where h denotes each of the observed DO estimates along the transect and σ^2 is a parameter that can be estimated from the data. Eq. (5) denotes the likelihood function for any single year; for all $g = 1$–29 years of available data the likelihood function is:

$$\prod_{g=1}^{29} \prod_{h=1}^{137} \frac{1}{\sqrt{2\pi\sigma^2}} exp \left[\frac{\left(DO_{gh} - DO_s + \frac{k_1 \times F \times BOD_u}{k_2 - k_1} \left(e^{-k_1 \frac{x_{gh}}{v}} - e^{-k_2 \frac{x_{gh}}{v}} \right) + D_i e^{-k_2 \frac{x_{gh}}{v}} \right)^2}{-2\sigma^2} \right]. \quad (6)$$

Scavia et al. (2006) held DO_s, k_1, and F constant across years at fixed values of 5 mg l^{-1}, 0.09 day^{-1}, and 0.85, respectively. The vertical flux parameter, k_2, was estimated using a salt-and-water-balance box model, adapted from Hagy et al. (2004), and applied to Chesapeake Bay by Hagy (2002). The resulting values that varied along the transect, were used for all years. Additionally, they used fixed *a priori* estimates of BOD_u and D_i, for each year. BOD_u and D_i were derived from the Susquehanna load and observed values at
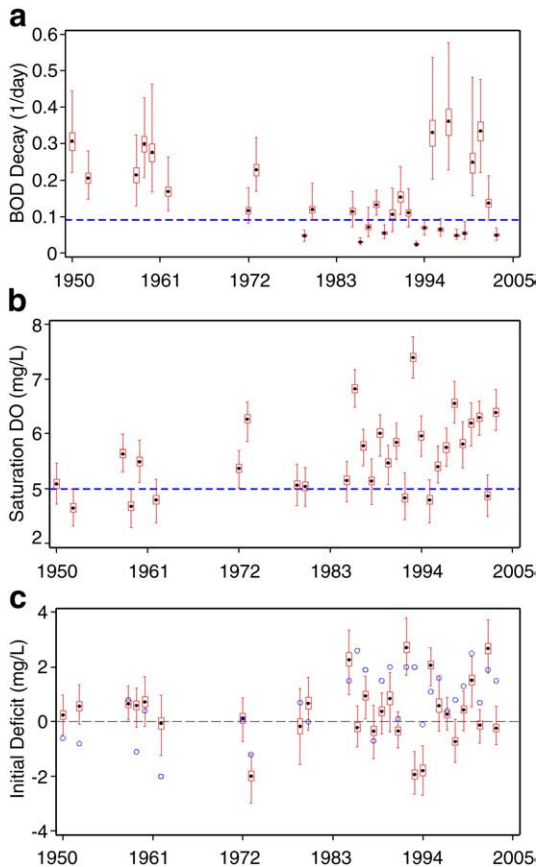
Fig. 2. Posterior distribution samples for each of the 29 years of available data for k_1 (a), DO_s (b), and D_i (c), with k_1, DO_s, and D_i independently estimated. Horizontal dashed blue lines indicate fixed values used by Scavia et al. (2006) for k_1 and DO_s; blue circles indicate values used by Scavia et al. (2006) for D_i. Dotted horizontal line at zero on D_i plots included for visual reference. Box and whisker icons depict posterior sample mean (black dot), median (horizontal red line in box), interquartile range (box), and extreme values (whiskers).

the model origin, respectively. In subsequent analyses, they used v as a calibration term and varied it among years to improve the model fit.

To demonstrate the utility of Bayesian approaches we start with the inputs used by Scavia et al. (2006) and systematically relax some of the fixed *a priori* assumptions, using the available data to estimate these inputs via Bayes Theorem. We impose a hierarchical structure on the model, allowing selected inputs to differ by year, with the assumption that the yearly estimates arise from a common normal distribution (Borsuk et al., 2001). The mean and variance of this "parent" normal distribution each require a prior distribution. We first allow k_1 to differ by year and estimate posterior distributions for all 29 years. Then we do the same for DO_s and estimate posterior distributions for each of the 29 years. Scavia et al. (2006) used fixed D_i values that differed across years; similarly we estimate D_i for all 29 years allowing it to differ by year. In each of these three demonstrations we use non-informative priors for the estimated model inputs. That is, we chose priors with large variance so that the posterior parameter distributions would effectively be determined by

the data, not by our *a priori* beliefs about plausible parameter values. For a fourth demonstration we simultaneously estimate k_1, DO_s, and D_i, allowing each of them to differ by year, again using non-informative priors for all of them. Finally, because estimating k_1, DO_s and D_i, simultaneously, results in unrealistic estimates for DO_s, we use a semi-informative prior distribution for DO_s (normal with mean = 5.0 and standard deviation = 0.167). This semi-informative prior places a loose *a priori* constraint on DO_s values, allowing the data to influence them, but keeping them in a physically plausible range. In all instances we use a non-informative prior distribution for model error variance σ^2.

3. Results

3.1. k_1, DO_s, and D_i independently estimated

When k_1 is estimated as a free parameter (Fig. 2a), most yearly k_1 values differ from the 0.09 value used by Scavia et al. (2006), though they vary about 0.09. Generally, k_1 decreases through time and the posterior precision (variance^{-1}) increases; however, four years late in the series (1995, 1999,
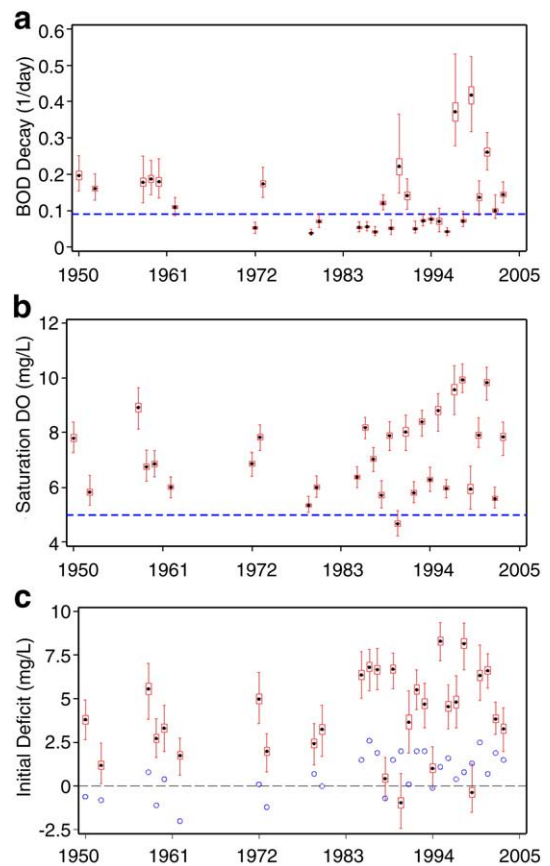

Fig. 3. Posterior distribution samples for each of the 29 years of available data for k_1 (a), DO_s (b), and D_i (c), with k_1, DO_s, and D_i jointly estimated. Horizontal dashed blue lines indicate fixed values used by Scavia et al. (2006) for k_1 and DO_s; blue circles indicate values used by Scavia et al. (2006) for D_i. Dotted horizontal line at zero on D_i plots included for visual reference. Box and whisker icons depict posterior sample mean (black dot), median (horizontal red line in box), interquartile range (box), and extreme values (whiskers).
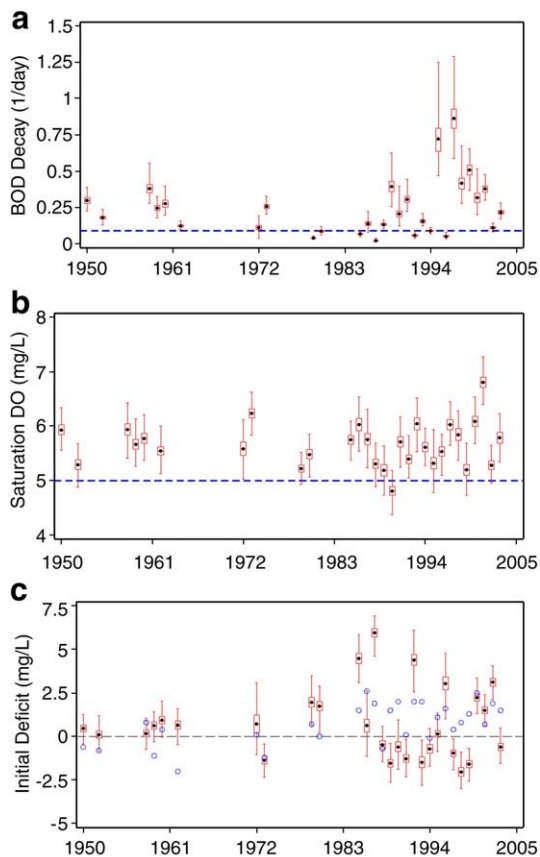
Fig. 4. Posterior distribution samples for each of the 29 years of available data for k_1 (a), DO_s (b), and D_i (c), with k_1, DO_s, and D_i jointly estimated and semi-informative prior distribution for DOs. Horizontal dashed blue lines indicate fixed values used by Scavia et al. (2006) for k_1 and DOs; blue circles indicate values used by Scavia et al. (2006) for D_i. Dotted horizontal line at zero on D_i plots included for visual reference. Box and whisker icons depict posterior sample mean (black dot), median (horizontal red line in box), interquartile range (box), and extreme values (whiskers).

2000, 2001) assume larger values with wider posterior distributions. The precision of the posteriors varies considerably among years; with k_1 precisely estimated in some years but with relatively high uncertainty in others. Most of the posteriors are asymmetric with slightly longer positive tails, though posterior means and medians tend to be approximately coincident. All estimates are consistent with plausible values reported for this coefficient (Bowie et al., 1985).

Similarly, when allowed to differ by year, DO_s (Fig. 2b) is generally higher than the 5.0 mg l^{-1} constraint imposed by Scavia et al. (2006). Estimates show an overall increase with time while the relative precision of the DO_s posteriors is more consistent than that of k_1. Posterior means range from ~4.8–7.5 mg L^{-1}, plausible for the salinity/temperature conditions of Chesapeake Bay.

Yearly D_i estimates also differ from imposed values (Fig. 2c), though the range of values among years is consistent with values used by Scavia et al. (2006). Generally, the earlier years tend to be higher than values used by Scavia et al. (2006) and the latter years tend lower. Like DO_s posterior precision for D_i is also fairly consistent across years in contrast to k_1.

3.2. k_1, DO_s, and D_i simultaneously estimated

Estimating k_1, DO_s, and D_i simultaneously reveals correlation among the three parameters (Qian et al., 2003). Most k_1 posterior means exhibit slight decreases over the years, and the precision of most of the k_1 posteriors increases (Fig. 3a), as compared to the estimates from estimating only k_1 (Fig. 2a). The pattern with time still displays a general decrease, with a few unusually high values late in the series.

Means for both DO_s and D_i exhibit marked increases over time (Fig. 3b and c, respectively), when compared to the estimates obtained when these inputs were individually estimated (Fig. 2b and c, respectively). DO_s and D_i are strongly positively correlated in this application; increases (or decreases) in one will tend to be accompanied by increases (or decreases) in the other. Conversely, DO_s and D_i are weakly negatively correlated with k_1. When estimated with k_1 and D_i, some DO_s posteriors assume values as high as ~11 mg l^{-1}, a physically unrealistic range given Chesapeake Bay salinity/temperature conditions. These unrealistic values result largely from the correlation among the three model inputs, a consequence of the mathematical structure of the model (Stow et al., 2007). Bayes theorem provides a convenient approach to this problem; instead of using a non-informative prior for DO_s, a semi-informative prior can be used, effectively imposing a loose constraint on DO_s. To "discourage" DO_s from attaining implausible values (Fig. 3b) we re-estimated k_1, $\underline{DO_s}$, and D_i simultaneously using a normal mean of 5.0 and standard deviation of 0.167 for the prior distribution of DO_s, capturing the *a priori* belief that DO_s values greater than ~5.5 mg l^{-1} are unlikely. With this constraint, k_1, DO_s, and D_i respond as expected; overall DO_s and D_i decrease and k_1 increases (Fig. 4a, b, c).

3.3. Model error variance

The model error term, ε, captures the component of DO variability that is not described by the Streeter–Phelps model, including observation error, and the error variance, σ^2, is an index of the magnitude of that un-described variation. Expressing this term as the model error standard deviation,
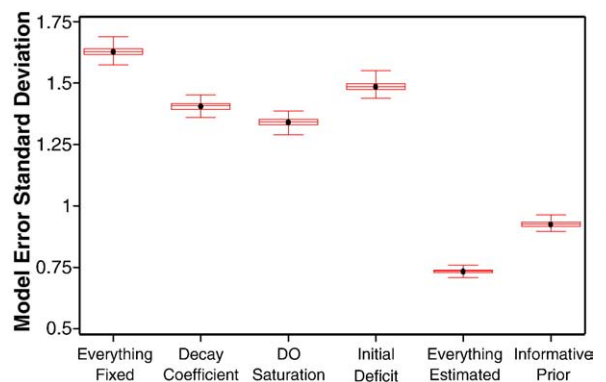

Fig. 5. Posterior distribution sample representing model error standard deviation (σ) with fixed inputs fixed used by Scavia et al. (2006), only k_1 estimated, only DO_s estimated, only D_i estimated, k_1, DO_s, and D_i simultaneously estimated with non-informative priors, and k_1, DO_s, and D_i estimated with semi-informative prior for DO_s.
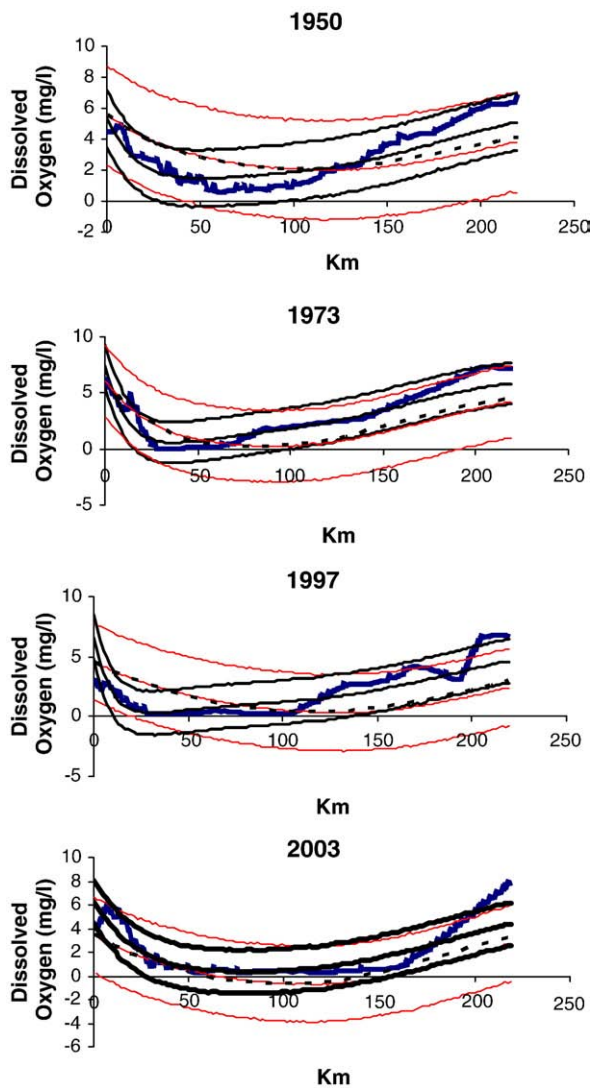
Fig. 6. Model predictions and observations (blue line) for representative years. The red dotted lines are the mean prediction and bounds of the 95% predictive interval from the model with fixed inputs. The solid dark lines are the mean prediction and bounds of the 95% predictive interval from the model with k_1, DO$_s$, and D_i estimated, and a semi-informative prior on DOs. The dashed line depicts predictions from the model used by Scavia et al. (2006).

σ, maintains the units in mg l^{-1} providing a more intuitive interpretation. With all parameters fixed, the posterior mean for $\sigma \sim 1.63$, indicating a high predictive uncertainty (Fig. 5). As the model fit to the observed DO data improves, by estimating various inputs, the posterior mean for σ decreases. With k_1 estimated, the posterior mean for σ drops to ~1.41; with DO$_s$ estimated, the posterior mean drops to ~1.34; and with D_i estimated, the posterior mean is ~1.48. However, the biggest decrease is realized when all three inputs are estimated. In that case, the posterior mean for σ declines to ~0.73. When the semi-informative prior is imposed on DO$_s$, the posterior mean for σ rebounds slightly to ~0.93.

Predictive uncertainty arises from a combination of the input uncertainty and the model error variance. Generally, predictive uncertainty decreases as more inputs are estimated

and the model error variance declines; however this decline in the model error variance is partially offset by the accompanying input uncertainty that arises when inputs are estimated rather than fixed. Fig. 6 compares model mean predictions and corresponding 95% predictive intervals from the model with fixed parameters and the model with the semi-informative prior for DO$_s$ for four representative years. In all cases the predictive interval width is greatly reduced when inputs are estimated instead of fixed, reflecting the decreasing model error variance (Fig. 5). Additionally, the mean predictions track the observed values better with estimated inputs because different values of k_1 and DO$_s$ were estimated for each year instead of using one value chosen to work acceptably well among all years.

4. Discussion

Ensemble estimation is based on the premise that, when multiple response variables share common or similar parameters, simultaneous estimation of these parameters yields more precise inference (Congdon, 2001), a result of "borrowing strength from the ensemble" (Morris, 1983). This idea has deep roots in the Bayesian literature (Box and Draper, 1965; Efron and Morris, 1972, 1973a) and underlies Empirical Bayes approaches (Efron and Morris, 1973b, 1975) as well as their closely-related, current incarnation as hierarchical/multilevel models (Gelman and Hill, 2007; Qian and Shen, 2007).

This approach represents a compromise. On one hand, a model developed using data from multiple years will probably be less accurate for a specific year, because the model represents the average of the years. On the other hand, a model based only on year-specific data will have a larger uncertainty because of the smaller year-specific sample size. Hierarchical models provide a rigorous methodology to systematically combine information from several sources and appropriately weight the group-specific or year-specific information depending on the degree of similarity to other groups in the data set.

In our application we somewhat arbitrarily chose three model parameters k_1, DO$_s$, and D_i to estimate as ensembles (within a hierarchical structure), differing by year but arising from a common parent distribution, while σ^2 was modeled to have the same value for all years. Many other combinations are possible, for example σ^2 could also be allowed to differ by year with (or without) a common parent distribution, or any of the model parameters could be estimated by assuming they are the same across years, differ by year but have a common hierarchical structure, or are independent from year to year (no hierarchical structure). However, allowing all the estimated parameters to independently differ by year, without a hierarchical structure, is equivalent to estimating each year separately and confers none of the benefit of ensemble estimation. Our intent in this presentation was largely to illustrate the methodological approach; we are continuing to experiment with the model by systematically altering the underlying assumptions and estimating different parameter sets. In our eventual application of this model we intend to examine differences in some of the parameters that have occurred through time, such as F and BOD$_u$ Most of the parameter time-trajectories presented herein (Figs. 2–4) reveal an increase in variance occurring in the mid-1980s, consistent with previous work that has suggested important changes in the

estuary occurred at approximately that time (Hagy et al., 2004; Kemp et al., 2005). These changes may indicate important ecosystem processes that have changed over time and provide clues for more effective management. Additionally, this model provides a basis to estimate the effect of future BOD reductions and the corresponding probabilities of attaining management goals (Borsuk et al., 2002). Future model improvements will also include incorporation of a lognormal model error to bound DO predictions at zero. The Bayesian approach can facilitate many different model error forms and other alternatives to a normal error structure may be considered as well.

Bayesian methods are sometimes criticized because they require subjective user-provided prior information. Berger and Berry (1988) countered this criticism, demonstrating that statistical inference is inherently subjective, often rather subtly. The use of expert judgment-based *a priori* fixed values for model parameters is common and well-accepted in environmental/ecological modeling, yet it is highly subjective. Our presentation reveals that Bayesian approaches allow reduced subjectivity by using imprecise *a priori* information thus, letting the observations more strongly influence inference. The semi-informative normal prior we used for DO_s with mean = 5.0 and standard deviation = 0.167 is consistent with the *a priori* belief that there is only a one percent chance that DO_s values fall outside the 4.5–5.5 mg l^{-1} range, yet many of the final estimates were outside the range (Fig. 2–4). This result illustrates that even with a relatively tight a priori constraint Bayesian methods can permit the data to be influential.

While Bayesian methods are sometimes criticized for subjectivity, empirical modeling is occasionally disparaged as "simple curve fitting" because the model is largely determined by observed data. Our results demonstrate that the Bayesian framework facilitates a combined modeling approach, allowing the simultaneous use of *a priori* fixed parameter values, semi-informative prior distributions, and non-informative priors. Thus, Bayesian modeling further facilitates the compromise modeling philosophy advocated by Scavia et al. (2006).

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