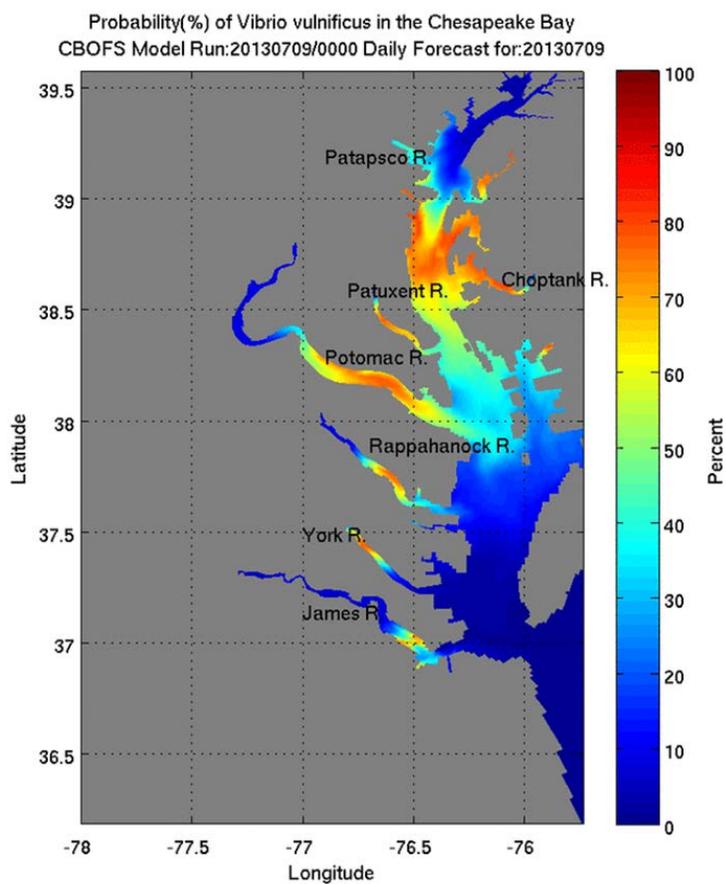


# Skill Assessment of NOAA's Chesapeake Bay *Vibrio vulnificus* Model October 2015



NOAA Technical Memorandum NOS NCCOS 215

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**For more information contact:** [John.Jacobs@NOAA.gov](mailto:John.Jacobs@NOAA.gov)

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## Skill Assessment of NOAA's Chesapeake Bay *Vibrio vulnificus* Model

**Lyon Lanerolle**  
NOAA NOS CSDL

**Robert Daniels**  
NOAA NWS NCEP OPC

**Bin Zhang**  
Cooperative Institute for Climate and Satellites  
University of Maryland

**John Jacobs**  
NOAA NCCOS Cooperative Oxford Laboratory

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United States Department  
of Commerce

**Penny Pritzker**  
Secretary

National Oceanic and  
Atmospheric Administration

**Kathryn D. Sullivan**  
Under Secretary  
of Commerce for  
Oceans and Atmosphere,  
and NOAA Administrator

National Ocean Service

**Russell Callender**  
Acting Assistant  
Administrator

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## EXECUTIVE SUMMARY

Since 2012, NOAA has generated model guidance for the probability of occurrence of the harmful marine bacteria *Vibrio vulnificus* in Chesapeake Bay. The system employs NOAA's Operational Forecast System for Chesapeake Bay (CBOFS) to force a statistical model developed by NCCOS and provides daily guidance for the entirety of the Bay. While the empirical model was validated in 2014, the system as a whole has not been assessed for model skill. In this memorandum, we report the results of a skill assessment conducted with paired observations and model predictions for the year 2011. As part of this exercise, we also evaluate model sensitivity to provide guidance on accuracy requirements for needed fields obtained from CBOFS.

Model sensitivity is dependent on the salinity in which predictions are applied. Bias in modeled salinity has a more pronounced effect in lower salinity areas (< 5PSU) than high. Overall, results suggest that effective criteria for accuracy requirements from CBOFS for this product are within 1°C and 1 PSU.

Predicted sea surface temperature (SST) was relatively close to requirements having an average difference between predicted and observed of 1.4°C. Modeled salinity, however, was positively biased by 2.5 PSU. This bias is a known issue with many of the operational forecast systems, and was corrected using a post – hoc approach for the *Vibrio vulnificus* model guidance.

Predicted probability of *V. vulnificus* occurrence matched well with observed overall, with no apparent spatial or temporal trends in error. However, the model error slightly exceeds our criteria of < 10% RMSE (11%) when raw salinity data is used from CBOFS due to the 2.5 PSU bias. When salinity is adjusted to remove bias, as is done routinely for guidance dissemination, the criteria is met.

This initial skill assessment provides evidence that the system is fully capable of providing accurate guidance given accurate input. Attention should be focused on improving CBOFS salinity estimates. Currently, post-hoc correction of salinity bias is required to meet skill criteria. The monitoring program enabling this evaluation of skill is ongoing, and subsequent skill assessments will be conducted regularly to ensure maintenance of model performance.

## INTRODUCTION

Bacteria belonging to the *Vibrio* spp. genus occur naturally in coastal regions around the globe. However, certain species and strains are capable of causing human illness. In the United States, there are estimated to be 80,000 illnesses a year, a trend that has continued to increase over the past decade (Newton et al. 2012). Primarily, these illnesses are caused by consumption of raw or undercooked seafood, and direct exposure to natural waters. It is estimated that health care costs in the US resulting from *Vibrio* exposure are over \$300 million annually with the majority linked to premature death from a single species, *Vibrio vulnificus* (Ralston et al. 2011).

*Vibrio vulnificus* is a gram-negative, flagellated, halophilic bacterium that is generally present in mesohaline waters when water temperature exceeds 15°C. While the total number of cases in the US is generally low (~100/yr), the gruesome nature of the illness and high case fatality rate (~30%) (Newton et al. 2012) has led to considerable concern among the public health community and shellfish industry. Cases are roughly split evenly between those obtained by ingestion of raw seafood and exposure to infected waters. While those with underlying medical conditions such as liver disease and immune disorders are at higher risk, wound infections are a common route of entry. These often result in severe bullous lesions leading in many cases to amputation or death in instances of sepsis (Jones and Oliver 2009). Such cases are increasingly being reported by the media with alarming titles (i.e., "In Chesapeake Bay waters warmed by summer sun, a deadly pathogen lies in wait", Washington Post, July 26, 2014). The result is often recreational avoidance that impacts local economies.

Since its discovery as a potential human pathogen in 1976 (Hollis et al. 1976), much effort has been placed on understanding the ecology of these bacteria. They are highly adaptive, and freely associate with a variety of biotic and abiotic surfaces including water, sediment, fish, shellfish, algae, and zooplankton (Depaola et al. 1994; Johnson et al. 2010; Maugeri et al. 2006; Turner et al. 2009). A variety of water quality parameters have been reported to correlate with *V. vulnificus* abundance including but not limited to water temperature, salinity, chlorophyll, nutrients, turbidity, pH and total bacteria (Lipp et al. 2001; O'Neill et al. 1992; Oliver et al. 1982; Pfeiffer et al. 2003; Randa et al. 2004; Wright et al. 1996). With the exception of water temperature, and to a lesser extent salinity, the relationship of these parameters to *V. vulnificus* abundance are inconsistent, owing perhaps to unique characteristics of individual environmental systems and study design. In general, growth and abundance is positively correlated with water temperature when greater than 15° C with a preference for mesohaline salinities (Lipp et al. 2001; Motes et al. 1998; Randa et al. 2004). However, *V. vulnificus* may be cultured from samples of higher salinity waters (> 25 PSU) (Maugeri et al. 2006; Oliver et al. 1983; Tamplin et al. 1982) which again may relate to regional differences in the ecology of the system or strains present. Thus regional variation may be of great importance in fully understanding the ecology of *V. vulnificus*.

In 2005, through NOAA's Oceans and Human Health Initiative, a small scale project was initiated to develop predictive algorithms for potentially harmful bacteria in Maryland's Coastal Bays. The project took advantage of existing water quality monitoring networks to collect samples and was largely successful in demonstration of concept in how partnership programs

could be used to develop predictive tools to greatly reduce the need for state monitoring while providing spatially and temporally explicit data for use in protection of human health (Jacobs et al. 2009). This successful demonstration led to further discussion with project partners, the Maryland Department of the Environment and Department of Health and Mental Hygiene, on expansion of the concept to Chesapeake Bay with a focus on tools to assist with *V. vulnificus* recreational exposure infections. In 2006, The Maryland Department of Natural Resources and Chesapeake Bay Program Partner institutions added *Vibrio* sampling to their long established water quality monitoring program and provided the samples to NOAA's Ocean Service's Cooperative Oxford Laboratory (COL) for analysis. In 2007, Virginia waters were added and roughly 150 samples were collected monthly covering the full spatial extent of the Chesapeake and tidal tributaries. By 2009, enough data was available to develop preliminary models with an emphasis on the use of explanatory variables that are capable of being observed or modeled in either real time or forecasted (E.g.; water temperature, salinity, chlorophyll, etc.)(Jacobs et al. 2010). An initial, logistic regression model providing probability of occurrence of *V. vulnificus* was forced by modeled output from the Chesapeake Bay Regional Ocean Modeling System (ChesROMS) resulting in the first guidance system (Brown et al. 2002). The system was constructed by researchers at NOAA and the University of Maryland Center for Environmental Science's Horn Point Lab and maintained in a demonstration mode at the NOAA Chesapeake Bay Office (NCBO). The system was provided to our state partners for evaluation through a hidden URL to discourage public viewing during this process. Full validation of the Chesapeake *V. vulnificus* empirical model was conducted in 2012 and later published (Jacobs et al. 2014). Also in 2012, the Chesapeake *V. vulnificus* system was started using output generated by the Ocean Service's Center for Operational Oceanographic Products and Services (CO-OPS) Chesapeake Bay Operational Forecast System (CBOFS) that runs operationally at NWS/National Centers for Environmental Prediction (NCEP), which affords greater resolution and reliability.

CBOFS is an operational implementation of the Regional Ocean Modeling System (ROMS) for the Chesapeake Bay and is the hydrodynamic component of the prediction system. This fully 3-dimensional sigma-coordinate model, with a horizontal resolution of 30 meters to 5 kilometers and 20 vertical levels, simulates the circulation and physical properties (temperature, salinity, density, velocity, and mixing) of the Bay. The prototype prediction system consists of the OFS's, the habitat model, and a suite of Linux shell, Perl, and MATLAB scripts. The *V. vulnificus* daily forecasts are dynamically generated using SST and SSS data extracted from the NetCDF output files generated by the CBOFS running on the OPC designated blades on the NCEP Compute Farm (a redundant set of virtualized servers running RedHat Enterprise Linux 6). The OFS NetCDF files are sent operationally by NWS/NCEP/NCO to the NCEP Compute Farm where MATLAB scripts create the resultant daily forecast images. The images are sent to the OPC web server and appear on the password restricted web page: [http://origin.opc.ncep.noaa.gov/restricted/Vibrio/daily/Vibrio\\_daily.shtml](http://origin.opc.ncep.noaa.gov/restricted/Vibrio/daily/Vibrio_daily.shtml)

While the modeled guidance has been available for quite some time, and the underlying algorithm has been validated, skill has not been assessed for the system as a whole. Thus error associated with CBOFS SST and SSS fields combined with inherent error of the empirical model could be compounding resulting in inaccurate predictions. Alternatively, error could be consistently biased in opposite directions, resulting in no change or improvement of model predictions. As part of the pathway to transition this model to an operational status within

NOAA, we have amassed a separate dataset to pair with gridded modeled predictions to assess model skill. In addition, we use this exercise to evaluate the sensitivity of the empirical model to deviations in SST and SSS for use in defining criteria for CBOFS for ecological forecasting.

## METHODS

Vibrio Observations - The same monitoring program used to develop the *V. vulnificus* algorithm has remained in place to present, affording ample data for skill assessment. However, 2011 was the last year that seasonal sampling occurred that was not used in development of the empirical model or validation. Since 2011, monitoring has necessarily been reduced to summer months due to budgetary constraints. Surface water samples (0.5-1 m depth) were collected by the Maryland Department of Natural Resources and Virginia Department of Environmental Quality's water quality monitoring programs, according to Chesapeake Bay Program protocols (USEPA 1996). Sterile polypropylene bottles (500 ml) were rinsed three times, filled with surface water from the sample station, and then placed immediately on wet ice. Two replicate bottles were collected at a subset of these stations as standard protocol of the water quality monitoring programs. All samples were frozen at -20°C until sampling was completed for the month. Samples were subsequently subjected to DNA extraction and amplification of the *V. vulnificus* *VvhA* gene for quantification of *V. vulnificus* as previously described in detail (Jacobs et al. 2014). For the purpose of this analysis, only qualitative (present/absent) data was used.

SST/SSS *in Situ* Observations - Since *V. vulnificus* samples are collected at the same time and location as water quality by state partners, Chesapeake Bay Program Data was used for each sampling event. Physical parameters were measured at 0.5 meter increments *in-situ* with a YSI datasonde (YSI Incorporated, Yellow Springs, Ohio, USA) at 40 stations from April – October representing the full spatial range of tidal waters (Figure 1). In addition, data from the remainder of 2011 for T and S was used for performing CBOFS model skill for these physical parameters.

CBOFS Model Output - In 2011, a significant salinity drift was recognized during the summer in the CBOFS output. In addition, 2011 model runs were not archived and unavailable for analysis. To remedy the salinity drift, the model was re-initialized using an improved set of initial conditions generated via an objective analysis procedure. Sampling locations for *V. vulnificus* and water quality observations were paired with the associated CBOFS model grid. T and S fields were averaged over the first meter and paired with associated water quality and *V. vulnificus* data for each sampling day.

Skill Assessment - Several approaches were used to evaluate model predictions against observed data. First, sea surface temperature (SST) and salinity (SSS) from the full year of data for each station were compared with CBOFS model predictions using linear regression and evaluated for fit, bias, and RMSE. These comparisons were plotted monthly as deltas for T and S for visual spatial analysis of the continuity of bias. Next, modeled T and S fields were used to drive the empirical *V. vulnificus* probability model. The probability of occurrence,  $P_{V_v}$  is calculated using the logistic regression equation:

$$P_{V_v} = \exp(A) / [1 + \exp(A)]$$

where  $A = 4.288 + (0.211 * T) - (0.272 * S_{opt})$  and  $S_{opt} = |S - 11.5|$ .

Here, T and S are respectively the water temperature and salinity measured in degrees Centigrade and PSU. These probabilities were then plotted spatially for both CBOFS and CBP data sets month by month (for summer, 2011) to visualize spatial patterns in bias. The delta in predicted vs observed was also examined for T, S, and  $P_{VV}$  by month, salinity category, and the interaction (ANOVA) to evaluate spatial and temporal trends in error. Salinity categories were: Tidal Fresh/Oligohaline (< 5 PSU), Mesohaline (5-18 PSU) and Polyhaline (> 18 PSU). Finally, to evaluate the ability of the empirical model to correctly predict probability of occurrence, CBOFS-generated and CBP-generated probabilities were binned by model predicted probability to the nearest 0.5 percent. In each probability bin, the observed frequency of occurrence was tabulated from the raw data. The two sets were then evaluated independently for model fit using linear regression.

Sensitivity of empirical model to SST and SSS deviations - The sensitivity of the empirical model to SST and SSS deviations is a critical factor in determining the accuracy requirements of the underlying hydrodynamic model (CBOFS). Using multivariate calculus, the corresponding errors in  $P_{VV}$ ,  $\Delta P$  were estimated for T and S biases in ranges  $\pm 2$  °C and  $\pm 3$  PSU respectively. Thereby, the additive effects of T and S deviations can be displayed and examined via a 2D heat map as shown below.

## RESULTS

Sensitivity Analysis - Bias in T and S has significant influence on modeled probability of occurrence, but is dependent on the direction. If both T and S are biased in the same direction, they tend to cancel each other out and have limited influence on predicted probability of occurrence as expected from the model formulation. However, if biased in opposite directions, error accumulates. Because of this interaction, if modeled SST and SSS were to remain within 1°C and 1 PSU bias intervals, probability errors would lie (approximately) within  $\pm 10\%$ ,  $\pm 7\%$  and  $\pm 5\%$  intervals (Figure 1) for SSS values of 5, 11.5 and 25 PSU respectively. Therefore, it is necessary for the models to predict lower salinity values relatively more accurately than the higher values.

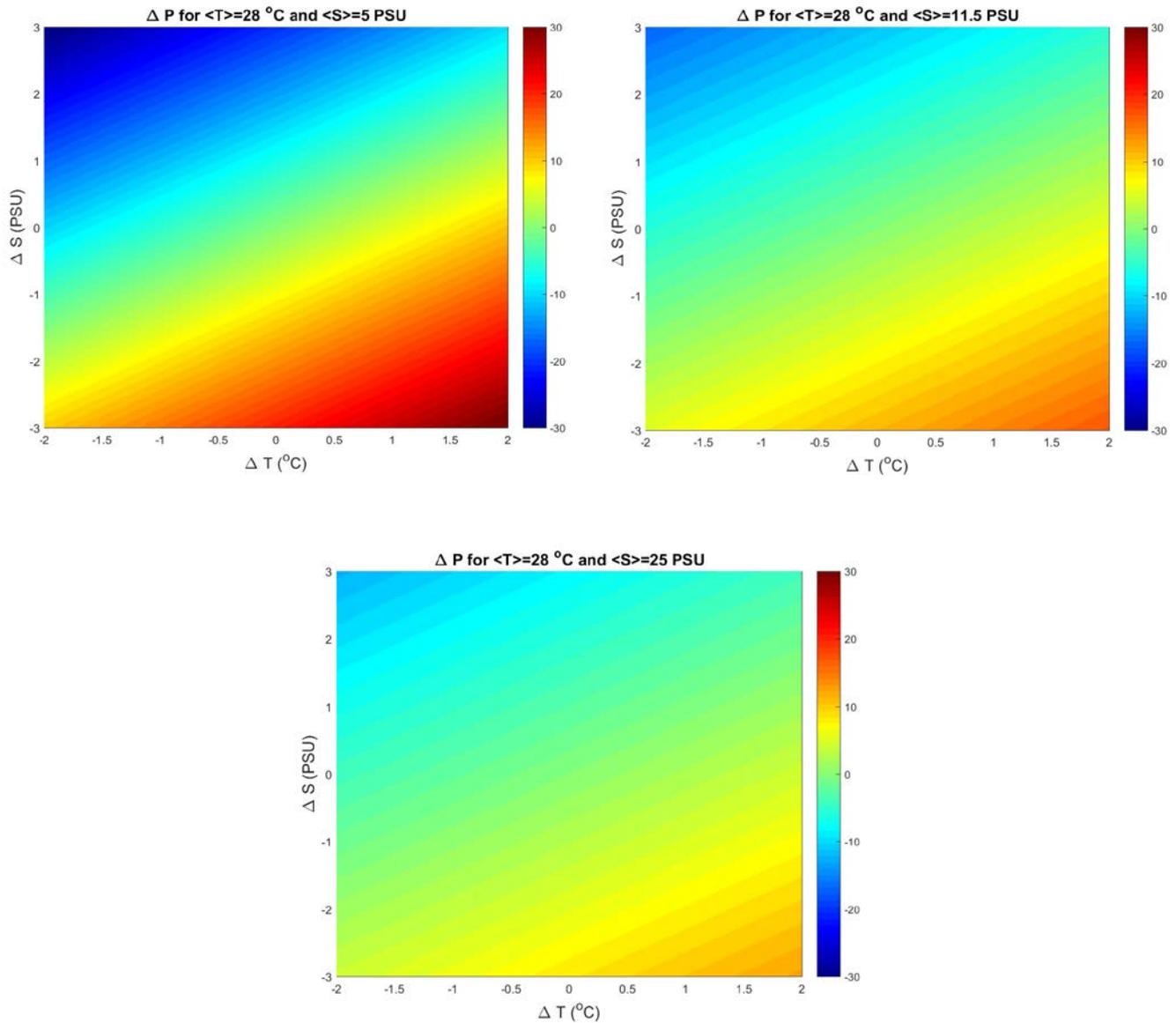


Figure 1. Sensitivity of  $P_{Vv}$  (% error) to SST and SSS errors about three mean (T, S) states. The temperature of 28 °C is kept fixed as it is a typical summer time value when *Vibrio* occurrence is observed. The three mean SSS values represent low, medium and high salinity scenarios. Note that the model becomes more robust with respect to SST and SSS error as salinity increases.

## Skill Assessment of the CBOFS predicted T and S

The skill assessment for SST is given in Figure 2 and for SSS in Figure 3. Overall, the CBOFS model predicted temperatures agreed well with observations. For the full year, the Root-Mean-Square (RMS) model-observation T difference was  $1.4^{\circ}\text{C}$  with a bias of  $+0.09^{\circ}\text{C}$  and a standard deviation of  $1.39^{\circ}\text{C}$ . Monthly spatial plots of the temperature difference like that for July, 2011 show that the model has good accuracy during the summer months when *Vibrio* are likely to be present. The corresponding plots for S in Figure 3 show that the modeled S was higher in value (saltier) than the observations with also greater scatter than for the T comparison. The RMS salinity difference for the full year of 2011 was 2.47 PSU with a bias of  $+1.28\text{ PSU}$  and standard deviation of 2.15 PSU. The salinity spatial error plots like that shown for July, 2011 exhibit a greater variation in value than temperature and hence, the main source of error in CBOFS is in its salinity predictions.

Spatial and temporal differences in error and the interaction were also examined for T and S. No significant differences were noted for temperature, suggesting that bias is equally distributed over the months sampled and does not change based on salinity category (Tidal Fresh/Oligohaline, Mesohaline, Polyhaline). Differences in predicted vs observed for salinity were not significant ( $P > .05$ ) for month or the interaction, but were for salinity category. Least square mean difference in predicted vs observed increased from 0.3 PSU in Tidal Fresh/Oligohaline waters, to 1.7 PSU in Mesohaline waters, to 2.1 in Polyhaline.

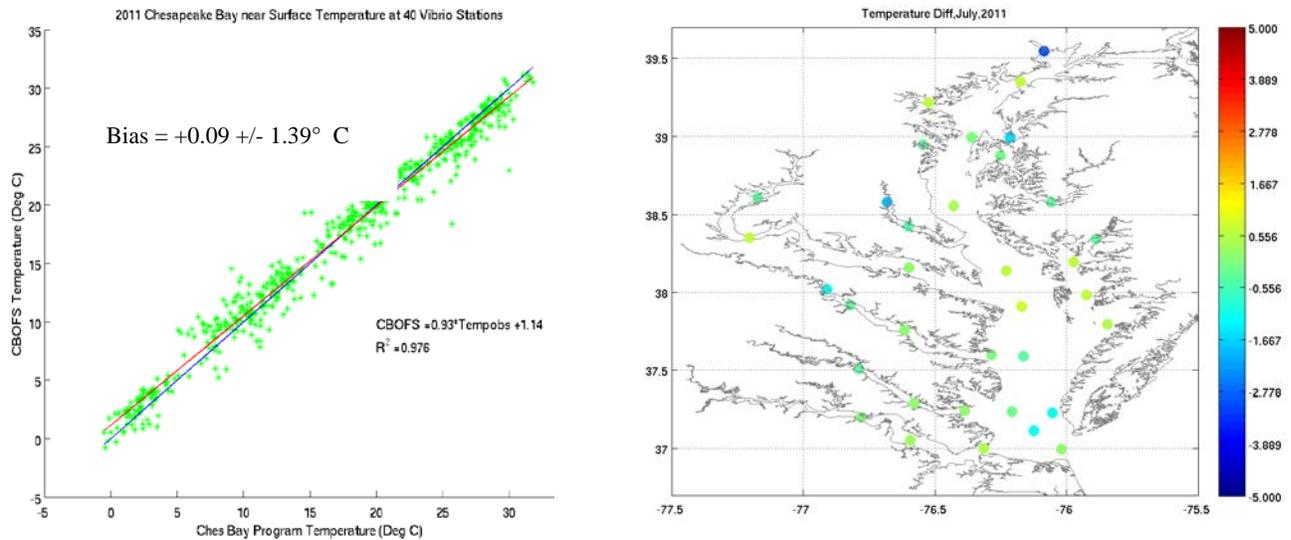


Figure 2. CBOFS versus observed SST comparison (left) where the blue line has a slope of 1 and the red line is the Least Squares fit. This comparison covers all 40 stations and for January –December of 2011. The T differences in space for July, 2011 are plotted in the second panel on the right.

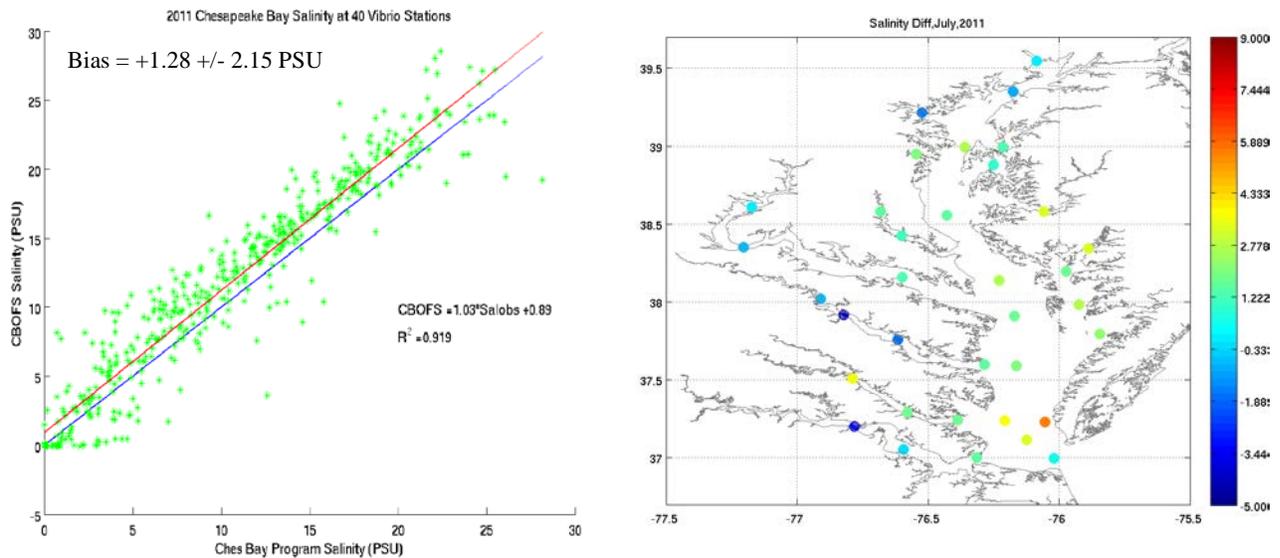


Figure 3. CBOFS versus observed SSS comparison (left) where the blue line has a slope of 1 and the red line is the Least Squares fit. This comparison covers all 40 stations and for January–December of 2011. The S differences in space for July, 2011 are plotted in the second panel on the right.

#### Probability of *V. vulnificus* occurrence from observations and model (CBOFS) predictions

Spatial comparisons were also made of the *V. vulnificus* probabilities calculated with CBP observations and CBOFS model predicted SST and SSS fields using the expression given in the Methods Section. Results for a typical summer month with high *Vibrio* probabilities, July 2011 is shown in Figure 4. As with temperature and salinity, error in predicted vs observed  $P_{VV}$  was evaluated with respect to temporal and spatial bias. Differences in predicted vs observed  $P_{VV}$  were not statistically significant even with the spatial bias in salinity. This is related to the model sensitivity as it is more robust to error at higher salinity than lower.

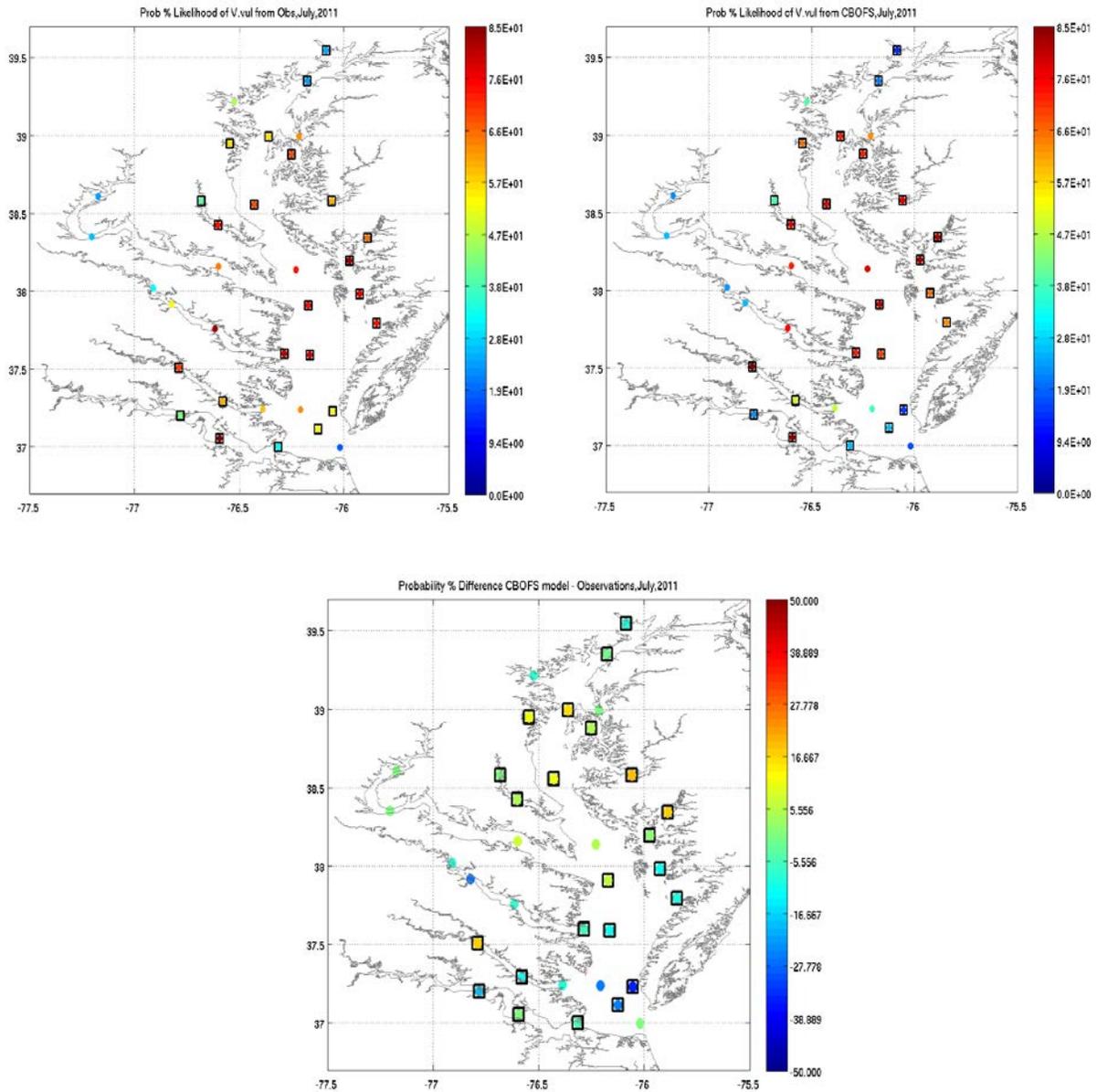


Figure 4. The probability of *V. vulnificus* occurrence in the form of a percentage calculated from CBP observations (top left), from CBOFS predicted T and S fields (top right) and the difference in probabilities based on CBOFS and CBP observations (bottom).

Our criteria for this initial skill assessment is that there would be less than 10% error in the model predicted probability. Most of the stations compared well with less than or close to a 10% difference in predicted probability, while 6 of the stations overpredicted the probability and 5 of the stations gave underpredictions. Black squares represent stations/locations where water bottle measurements generated a presence for *V. vulnificus*. Usually, the black squares agreed with predicted probabilities of greater than 50% in value. Stations which showed large differences in predicted probability were best explained by examining the probability sensitivity plot given in

Figure 1 where close to the optimal salinity of 11.5, a small error in salinity can lead to larger errors in probability. It can also be seen that if salinity and temperature errors act in the same direction, there is a cancelling effect and smaller probability errors result.

The probability of occurrence from the CBOFS T and S predictions was compared with the observed frequency of *V. vulnificus*, in order to test the end to end capability and the error of the full model (model-observations errors plus the errors in the  $P_{Vv}$  formulation). Observations were binned in intervals of 0.1 from 0 to 1.0, based on their predicted probability from the CBOFS T and S predictions (Figure 5, left panel). The observed frequency was calculated from the fraction of measurements within each bin that showed a presence of *V. vulnificus*. The predicted probability from CBOFS showed an 11 % RMS difference with the observed frequency. The predicted probabilities compared very well in the 0.55, 0.65 and 0.75 bins but showed larger differences with underpredictions in the 0.85 bin and over predictions in the 0.45 bin. When calculating probabilities based on observed salinity and CBOFS temperature (Figure 5, right panel) there was an improvement of 2 % in the error, shown in the new RMS of 9.2 % and in the closer fits of the 0.45 and 0.85 bins

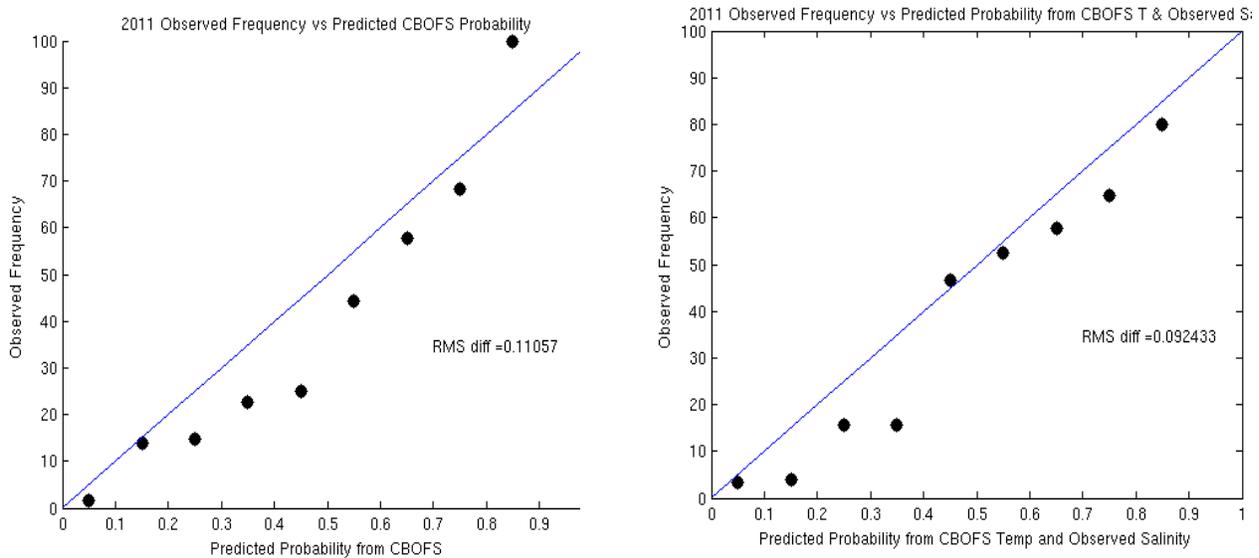


Figure 5. Binned observed Frequency of *V. vulnificus* versus the predicted model probability of occurrence from CBOFS predicted T and S (left) and CBOFS predicted T and observed S (right).

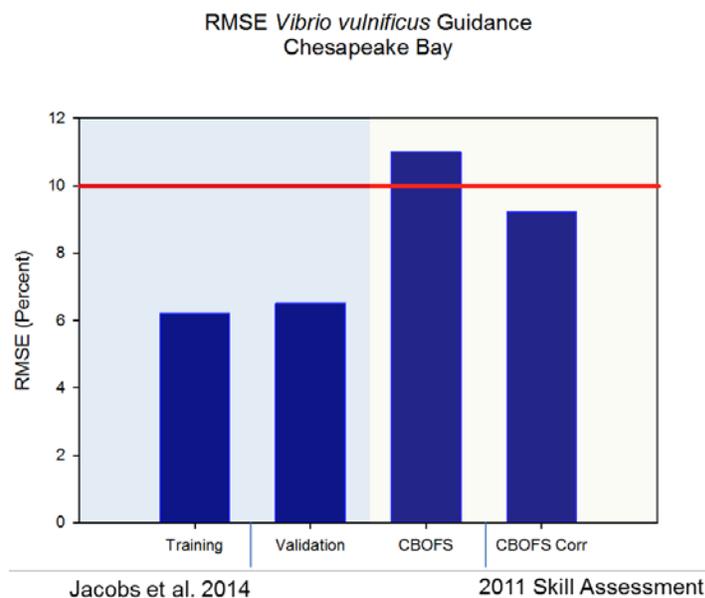


Figure 6. Comparison of RMSE from model development (training and validation data sets) and with using CBOFS input directly and corrected for salinity (CBOFS Corr).

## Discussion

This exercise served to address several pressing unanswered questions regarding the accuracy of the Chesapeake Bay *Vibrio vulnificus* modeled guidance. First, we addressed requirements for accuracy of CBOFS generated T and S and found that 1 PSU and 1°C are necessary to meet our stated goal of < 10% error in predicted probability. These values will be put forth through the EFR Infrastructure and Process as well as Modeling Team as EFR requirements of COOPS OFS models for ecological forecasting. Second, we found that CBOFS T predictions are adequate for our purposes, while S is not – especially the lower S predictions which influence the accuracy of  $P_{Vv}$  to a greater extent. Finally, given corrected salinity, the model is capable of performing adequately and within predefined criteria.

We used data collected in conjunction with state water quality monitoring programs from 2011 for this initial skill assessment in order to evaluate performance within a single year. Samples are available from later years, but the monitoring program was reduced to just 2 months of the year after 2011, providing far less data. The amount of data is of particular significance for the methods used to evaluate model skill when the data is binary. For each given probability level, the observations are binned for comparison. Therefore, it is necessary to have sufficient numbers of observations for each bin in order to accurately evaluate model performance. This likely accounts for some of the difference between the original empirical model validation and the CBOFS 2011 evaluation (Figure 6). In the next skill assessment, all data will be included to evaluate the influence of sample size on model skill.

It is clear from the skill assessment that in order to maintain less than 10% error on modeled guidance, salinity inputs from CBOFS need to be more precise. In our current mode of operations, we use real-time observations from the Chesapeake Bay Interpretive Buoy System (CBIBS) to correct salinity post-hoc on a bi-weekly basis. This process has allowed us to

maintain less than 1PSU bias, and should translate into less than 10% error in the model overall as demonstrated here. While use of data assimilation is promising and serves as a convenient fix, it does not address the underlying issue within CBOFS. In order to meet model requirements for ecological forecasting, improvements in CBOFS model skill or perhaps a more permanent strategy for data assimilation are warranted.

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United States Department of Commerce  
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