Supplement of Temporally resolved coastal hypoxia forecasting and uncertainty assessment via Bayesian mechanistic modeling

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Supporting information

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S1 DMO20 model description

DMO20 model, fully described in Del Giudice et al. (2020), is based on a steady-state solution to mass balance
differential equations presented in Obenour et al. (2015). Using time-varying inputs, DMO20 predicts daily BWDO \( (O_b) \) concentration (mg/L) from 1 June to 30 September of each year:

\[
O_b = \frac{(k_a O_b - D_w)}{k_a - D_s/O_f} - 1 \tag{S1.1}
\]

where \( k_a \) is the reaeration rate (m/d), \( D_w \) is the water column oxygen demand (WCOD), and \( D_s \) is the sediment oxygen demand (SOD) at \( O_f \), a reference oxygen concentration set to 3 mg/L.

The net WCOD (g/m²/d) of each lower compartment is represented as:

\[
D_w = J \gamma \omega = \left( \frac{L_r + L_u}{Q_r + Q_u + Q_g + \gamma + A} \right) \gamma \omega . \tag{S1.2}
\]

Here, \( J \) is the downward carbon flux (g/m²/d), \( \gamma \) is the mass ratio of oxygen demand to organic carbon set to 3.5, \( \lambda \) is the ratio of organic carbon to nitrogen set to 5.68, \( A \) is the area of the shelf section (Gm²), \( \omega \) is an oxygen demand adjustment factor (accounting for photosynthesis, off-shelf losses, etc.), and \( \nu \) is the effective settling velocity (m/d), which incorporates both the production and sinking of organic matter. The variables \( Q \) and \( L \) represent the near-term flows (Gm³/d) and N loads (Gg/d) entering the surface-layer model compartments, respectively. Subscripts \( r \), \( u \), and \( g \) denote the origin of these fluxes: Mississippi and Atchafalaya Rivers, upstream (i.e., eastern) shelf section, and the greater Gulf of Mexico. \( Q_g \) is approximated as a dilution factor (3.2, derived from surface salinity data) multiplied by mean Mississippi River discharge (1.6 Gm³/d).

The reaeration rate for each section is determined as a function of wind stress (representing shear-induced
turbulence) and freshwater flow (representing buoyancy):

\[
k_a = \beta_0 + \beta_1 \frac{U^2}{Q_s} \frac{A}{10000} \tag{S1.3}
\]

where \( U \) is the 14-day weighted mean wind speed for the shelf section (m/s), \( Q_s \) is the river discharge entering the section (Gm³/d), and \( \beta_0 \) and \( \beta_1 \) are calibration parameters.

Partitioning of riverine inputs is computed through:

\[
F_W = 0.5 - \beta_e v_e \tag{S1.4}
\]
where $F_w$ is the fraction of abovementioned flows and loads transported westward over the shelf, $v_e$ is the mean eastward wind velocity (m/s), and $\beta_e$ is a calibration parameter. The 0.5 indicates that, in absence of wind, inputs from both rivers would equally partition westward and eastward.

SOD is represented as:

$$D_s = B \sqrt{\frac{L}{L}} \theta^{T-\bar{T}}.$$  \hspace{1cm} (S1.5)

where $L$ (Mg/mo) is the combined nutrient loading from the Mississippi and Atchafalaya Rivers, averaged November-March. We normalize these pre-spring loads relative to their long-term average ($\bar{L}$) for the study period. SOD is temperature dependent and is based on the Arrhenius model with $\theta = 1.07$. Rates are corrected when temperatures deviate from $\bar{T}$, the summertime average. Here, $T$ is the monthly mean temperature.

A quadratic polynomial function $g$ is used to transform modelled bottom water dissolved oxygen (mg/L) into hypoxic area (km$^2$). For each section of the shelf, west and east, $g$ is:

$$HA_{West} = g(BWDO_{West}) = 62628 - 21353 \times BWDO_{West} + 1839 \times BWDO^2_{West}$$  \hspace{1cm} (S1.6)

$$HA_{East} = g(BWDO_{East}) = 17436 - 5945 \times BWDO_{East} + 507 \times BWDO^2_{East}$$  \hspace{1cm} (S1.7)

For Eq. S6 the $R^2 = 0.98$ and the residual standard deviation is 706 km$^2$, while for Eq. S7 the $R^2 = 0.99$ and the residual standard deviation is 216 km$^2$.

Table S1: Summary of the DMO20 model parameters estimated through Bayesian inference, including mean and 95% credible interval of each parameter.

| Parameter | Units | Description                          | 2.5%  | Mean  | 97.5%  |
|-----------|-------|--------------------------------------|-------|-------|--------|
| $v$       | m/d   | effective settling velocity          | 0.105 | 0.218 | 0.360  |
| $\omega$  | —     | oxygen demand adjustment factor      | 0.074 | 0.184 | 0.368  |
| $\beta_0$ | m/d   | reaeration parameter                 | 0.108 | 0.168 | 0.246  |
| $\beta_1$ | —     | reaeration parameter                 | 0.228 | 0.342 | 0.468  |
| $B$       | g/m$^2$/d | average sediment respiration rate | 0.225 | 0.335 | 0.446  |
| $\beta_e$ | m/m   | east-west advection coefficient      | 0.152 | 0.177 | 0.197  |
| $\sigma_{m,w}$ | mg/L | model error, west       | 0.289 | 0.375 | 0.460  |
| $\sigma_{m,e}$ | mg/L | model error, east       | 0.274 | 0.342 | 0.421  |
**S2 Bias adjustment for model predictions in June**

Preliminary analysis indicated that hindcasted BWDO was somewhat lower than observations for the west section of the shelf in June. This bias remained after conversion of BWDO to HA. A linear regression with zero intercept and a sequence of numbers 29 to 0 representing period from June 1 to June 30 as the predictor was used to estimate a bias adjustment, defined as difference between average observed and hindcasted BWDO divided by hindcasted BWDO. The resulting regression indicates a gradual decline in bias from the beginning of June (Fig. S2.1). The bias adjustment increases the $R^2$ of relationship between observed and hindcasted BWDO from –0.15 to 0.36 (Fig. S2.2), and between observed and hindcasted HA from –0.14 to 0.45 (Fig. S2.3).

![Figure S2.1](image)

**Figure S2.1:** Bias adjustment factor vs day number (before 1 July) for the west section with red line showing the regression fit with slope mean and standard error of 0.007 and 0.001, respectively. The adjusted $R^2$ of this regression is 0.20.
Figure S2.2: Month by month comparison of observed with hindcasted (black) and bias-adjusted hindcasted (red) averaged BWDO in the west and east sections. Diagonal lines represent perfect prediction.

Figure S2.3: Month by month comparison of observed with hindcasted (black) and bias-adjusted hindcasted (red) averaged HA in the west and east sections. Diagonal lines represent perfect prediction.
S3 Regressions for predicting summer Mississippi and Atchafalaya River flow and loading

Figure S3.2: Observed versus predicted by regressions square-root transformed Atchafalaya River monthly average discharge. Subscript numbers indicate months (June-September).
Figure S3.3: Observed versus predicted by regressions square-root transformed Atchafalaya River monthly average nitrogen loading. Subscript numbers indicate months (June-September).
Figure S3.4: Observed versus predicted by regressions square-root transformed Mississippi River monthly average discharge. Subscript numbers indicate months (June-September).
Figure S3.5: Observed versus predicted by regressions square-root transformed Mississippi River monthly average nitrogen loading. Subscript numbers indicate months (June-September).
| Year | Jun (m³/s) | Jul (m³/s) | Aug (m³/s) | Sep (m³/s) | Jun (t/mo) | Jul (t/mo) | Aug (t/mo) | Sep (t/mo) |
|------|------------|------------|------------|------------|------------|------------|------------|------------|
| 1980 | 6267       | 5860       | 4719       | 4130       | 3429       | 3270       | 3466       | 3410       |
| 1981 | 7743       | 8970       | 5517       | 6360       | 3872       | 4870       | 2699       | 3390       |
| 1982 | 8692       | 8820       | 7035       | 6220       | 4148       | 4270       | 3805       | 4030       |
| 1983 | 13167      | 15200      | 6754       | 6100       | 5385       | 3450       | 3088       | 1880       |
| 1984 | 8963       | 9990       | 5293       | 6010       | 4229       | 3740       | 3273       | 2050       |
| 1985 | 5756       | 5670       | 4409       | 3980       | 3270       | 2860       | 3630       | 3270       |
| 1986 | 6284       | 7650       | 4550       | 5070       | 3434       | 3010       | 2756       | 2570       |
| 1987 | 6180       | 4710       | 5014       | 3820       | 3401       | 2520       | 2725       | 2460       |
| 1988 | 3175       | 2130       | 2972       | 1480       | 2406       | 1540       | 3427       | 1530       |
| 1989 | 6758       | 8310       | 5372       | 8520       | 3579       | 3560       | 3340       | 3960       |
| 1990 | 10735      | 13500      | 8260       | 6890       | 4724       | 4310       | 2673       | 3690       |
| 1991 | 11184      | 9240       | 7418       | 4590       | 4849       | 2840       | 2874       | 2510       |
| 1992 | 3628       | 4920       | 3084       | 4780       | 2568       | 5900       | 2587       | 3500       |
| 1993 | 9887       | 9120       | 5878       | 8220       | 4490       | 9690       | 3639       | 6560       |
| 1994 | 6458       | 5220       | 4147       | 4740       | 3489       | 3480       | 3436       | 2810       |
| 1995 | 12495      | 13300      | 8971       | 7610       | 5202       | 4750       | 3146       | 2960       |
| 1996 | 9797       | 11700      | 6038       | 5810       | 4463       | 4790       | 3692       | 3290       |
| 1997 | 7001       | 9140       | 5553       | 6520       | 3653       | 3530       | 3401       | 2770       |
| 1998 | 6777       | 7330       | 4941       | 8150       | 3586       | 4760       | 2902       | 2730       |
| 1999 | 8043       | 6930       | 6262       | 6220       | 3961       | 3430       | 2829       | 2150       |
| 2000 | 5037       | 5080       | 4519       | 5980       | 3040       | 3090       | 2705       | 2220       |
| 2001 | 6556       | 8080       | 5494       | 4720       | 3517       | 3370       | 3269       | 2690       |
| 2002 | 8433       | 9680       | 5380       | 3940       | 4075       | 2870       | 3128       | 2700       |
| 2003 | 8552       | 8800       | 5918       | 5370       | 4108       | 4260       | 3272       | 3760       |
| 2004 | 8394       | 9440       | 6616       | 7750       | 4062       | 3870       | 3053       | 4090       |
| 2005 | 4412       | 4400       | 4324       | 3540       | 2835       | 2270       | 2904       | 2940       |
| 2006 | 4285       | 3650       | 3887       | 2770       | 2793       | 2140       | 2601       | 2270       |
| 2007 | 7123       | 4880       | 5863       | 5830       | 3689       | 3620       | 3205       | 5350       |
| 2008 | 11507      | 9760       | 7449       | 8550       | 4937       | 5010       | 3460       | 5560       |
| 2009 | 9380       | 11200      | 5754       | 5670       | 4347       | 4800       | 3232       | 3910       |
| 2010 | 9360       | 8380       | 6209       | 7240       | 4339       | 5640       | 3325       | 3940       |
| 2011 | 14625      | 12700      | 8231       | 7390       | 5770       | 4610       | 3474       | 3670       |
| 2012 | 4256       | 2790       | 4230       | 2130       | 2783       | 1800       | 2303       | 1870       |
| 2013 | 10871      | 9810       | 7915       | 7710       | 4762       | 4550       | 3486       | 2730       |
| 2014 | 6012       | 7090       | 4552       | 6010       | 3350       | 3550       | 3821       | 3940       |
| 2015 | 13207      | 10500      | 9104       | 12700      | 5393       | 8150       | 3180       | 2820       |
| 2016 | 7966       | 7280       | 6164       | 4790       | 3939       | 5070       | 2682       | 4280       |

Table S3.1: Predicted by the regressions (pre) and observed (obs) monthly Atchafalaya River discharge and nitrogen loading.
| Year | Mississippi River | Loading (t/mo) |
|------|------------------|---------------|
|      | Jan   | Feb   | Mar   | Apr   | May   | Jun   | Jul   | Aug   | Sep   | Oct   | Nov   | Dec   |
| 1980 | 14630 | 13600 | 11343 | 9490  | 8135  | 7860  | 8274  | 8010  | 63302 | 65152 | 47753 | 41706 | 26594 | 28307 |
| 1987 | 14341 | 12726 | 11082 | 9260  | 7762  | 7550  | 8034  | 7330  | 63122 | 57531 | 46965 | 32609 | 26875 | 19074 |
| 1991 | 14582 | 17700 | 11759 | 11800 | 8115  | 7530  | 6669  | 6360  | 80192 | 112690 | 59026 | 63614 | 32276 | 28958 |
| 1996 | 15749 | 20120 | 12198 | 19900 | 8475  | 8400  | 7990  | 9310  | 60823 | 60366 | 47985 | 48845 | 25237  | 15385 |
| 2000 | 14581 | 22070 | 17243 | 15050 | 11552 | 6667  | 9367  | 6260  | 137626 | 126306  | 95863  | 50828 | 51343  | 24382 |
| 2004 | 15744 | 19200 | 12198 | 19900 | 8475  | 8400  | 7990  | 9310  | 60823 | 60366 | 47985 | 48845 | 25237  | 15385 |
| 2008 | 15744 | 19200 | 12198 | 19900 | 8475  | 8400  | 7990  | 9310  | 60823 | 60366 | 47985 | 48845 | 25237  | 15385 |
| 2012 | 15744 | 19200 | 12198 | 19900 | 8475  | 8400  | 7990  | 9310  | 60823 | 60366 | 47985 | 48845 | 25237  | 15385 |

Table S3.2: Predicted by the regressions (pre) and observed (obs) monthly Mississippi River discharge and nitrogen loading
S4 Forecast skill and variance assessment

Figure S4.1: Daily hindcasted HA and observed HA versus pseudo-forecasted HA for the west and east sections. Diagonal line represents perfect prediction.

Figure S4.2: Averaged daily variance of total HA due to different sources of uncertainty. In this case, the “residual error” variance includes transformation and bias uncertainties, in addition to the DMO20 residuals. Note that the relative magnitudes of the variance components are somewhat different from the magnitudes of the IQR components (e.g., Fig. 5) because variance has squared units.
Figure S5.1: Daily pseudo-forecasts of HA for the west and east sections in 1985 (top) and 1986 (bottom), including 95% IQR of the predictive distribution, distinguishing between i) parameter, ii) hydrometeorological inputs, iii) mechanistic model error, and iv) regressions related to transformation of BWDO to HA and bias adjustment uncertainties (shades of gray from lightest to darkest). Yellow dashed line is hindcasted estimate, black dashed line is the 32-year average hindcast, orange points and error bars represent the mean and associated 95% confidence interval of the (geostatistically estimated) hypoxia observations.
Figure S5.2: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.3: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.4: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.5: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.6: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.7: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.8: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.9: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.10: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S5.11: Pseudo-forecast as in Fig. S5.1 but for different years.
Figure S6.1: Daily pseudo-forecasts of total HA, including 95% IQR of the predictive distribution (1985-1988), distinguishing between i) parameter, ii) hydrometeorological inputs, iii) mechanistic model error and iv) regressions related to transformation of BWDO to HA and bias adjustment uncertainties (shades of gray from lightest to darkest). Yellow dashed line is hindcasted estimate, black dashed line is the 32-year average hindcast, orange points and error bars represent the mean and associated 95% confidence interval of the (geostatistically estimated) hypoxia observations.
Figure S6.2: Pseudo-forecast as in Fig. S6.1 but for different years.
Figure S6.3: Pseudo-forecast as in Fig. S6.1 but for different years.
Figure S6.4: Pseudo-forecast as in Fig. S6.1 but for different years.
Figure S6.5: Pseudo-forecast as in Fig. S6.1 but for different years.
Figure S6.6: Pseudo-forecast as in Fig. S6.1 but for different years.
Figure S6.7: Pseudo-forecast as in Fig. S6.1 but for different years.
Figure S6.8: Pseudo-forecast as in Fig. S6.1 but for different years.
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