Water Column Oxygen Anomalies in the Aftermath of the BP Oil Spill

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Introduction

The 2010 Macondo oil spill injected an unprecedented amount of hydrocarbons into Gulf of Mexico deep waters. A poorly constrained fraction of this reduced carbon input dispersed in the water column.

As the biological breakdown of reduced hydrocarbons consumes O_2, depletion of this electron acceptor may indicate the past presence of hydrocarbons. Here, we present our attempts to quantify O_2 anomalies from a sparse data set using multivariate splines in 2 dimensions. We compare and contrast these results with those from alternative interpolation methods such as ordinary kriging.

Data

We used O_2 concentration profiles collected on NOAA ship Pisces Cruise IV between August 19 and September 2, 2010, predominantly southwest of the Deepwater Horizon drill site. From these observational data, O_2 anomalies were quantified by manually curating measured profiles and identifying O_2 depletion against background concentrations in approximately 1 m depth intervals between 700 m and 1300 m water depth (Figure 1).

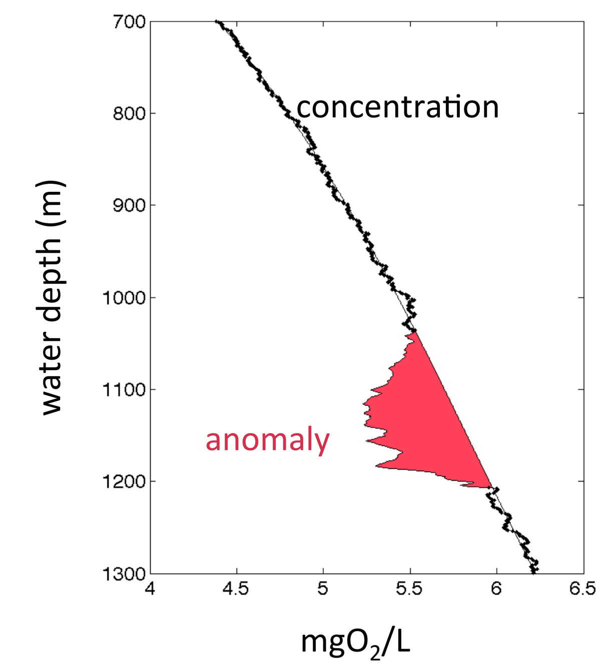

Figure 1: Example of O_2 profile & anomaly

A total of 131 profiles were used, giving rise to the distribution of O_2 depletion shown in Figure 2. Despite the comparatively larger number of measured profiles, the sparse nature of the dataset makes the quantification of the total O2 drawdown challenging. We approach this issue by applying a novel bivariate spline methodology. We first apply it to high-resolution model data to optimize the parameterization, and then use it to interpolate the data set shown in Figure 2.

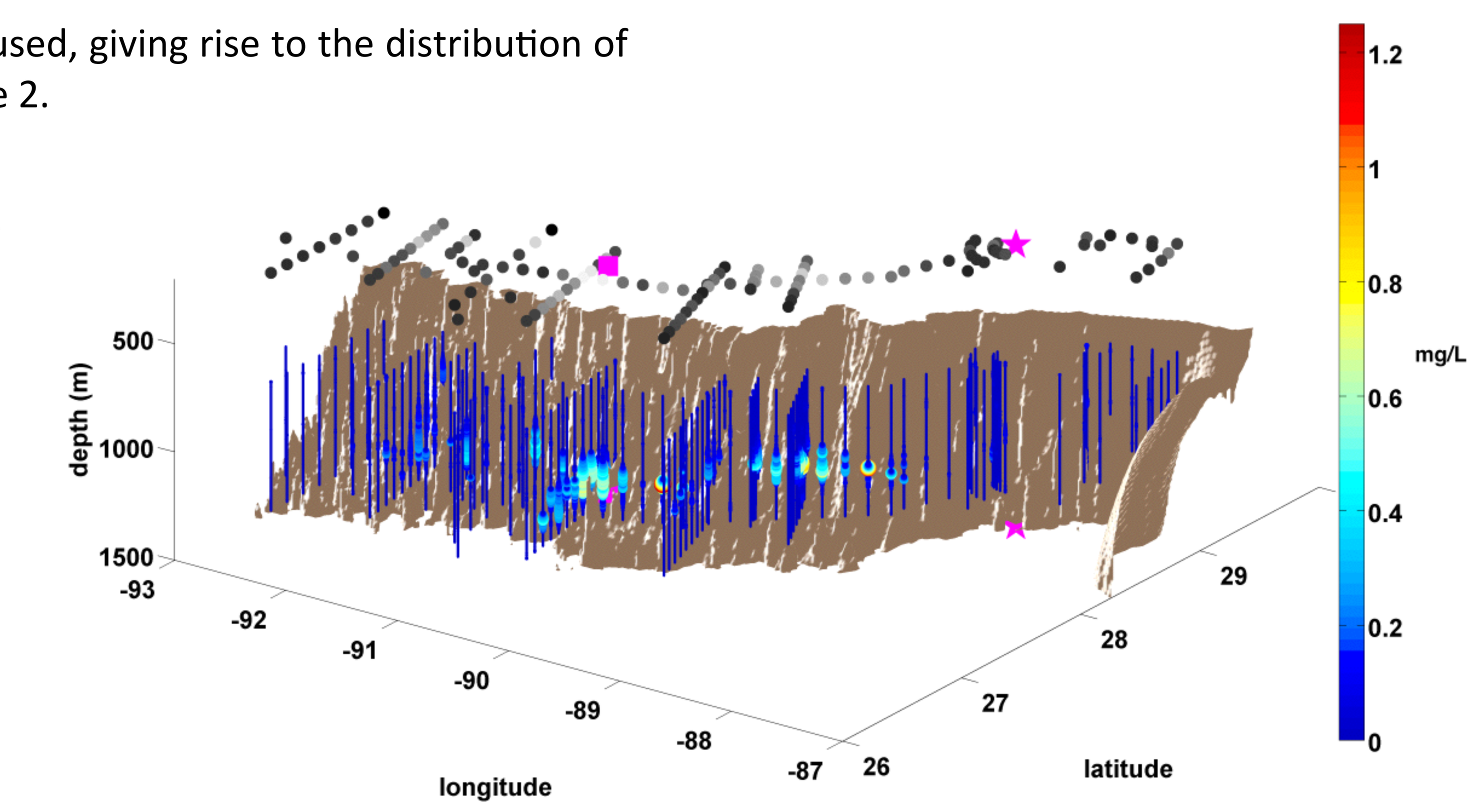

Figure 2: Spatial distribution of O_2 anomalies (Joye et al. 2011)

Approach

Our computation of the total amount of O_2 depletion from the data collected over the two-week period of Pisces cruise IV entails

1. Computation of a bivariate spline fitting function over the given data values for each depth layer.
2. Integration of each fitting function across the domain and summation over the contribution from each layer.

We implemented this algorithm in MATLAB based on Awanou et al. (2006).

First, we created a well-conditioned triangulation covering the locations where data values were measured (Figure 3), and then determine bivariate splines as outlined in Box 1.

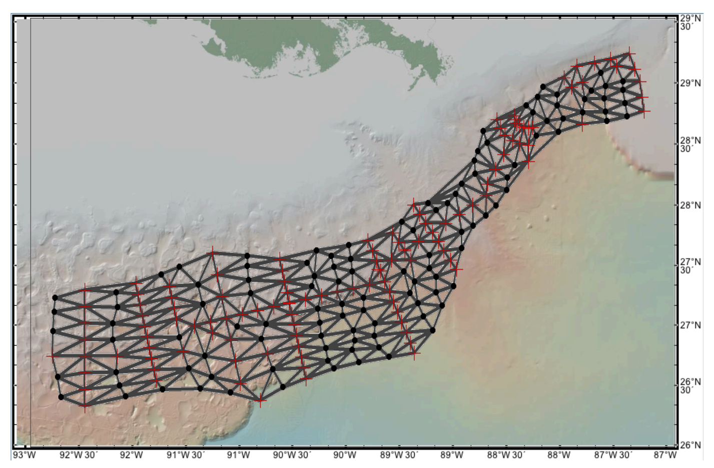

Figure 3: Profile locations (red crosses) and additional triangulation vertices (black dots).

In addition to the bivariate splines, we also used ordinary kriging to interpolate O_2 anomalies between measurements. An exponential model was fitted to the empirical variogram; nugget, sill and range was determined either from the high-resolution model simulations or – for each layer – from the measured profiles.

Box 1: Bivariate spline methodology

Let $S^r_d(\triangle)$ be the spline space of degree d, smoothness $r \geq 1$ with $d > r$ over triangulation $\triangle$. For example, $d = 5$ and $r = 1$. For each layer j we compute $S_j \in S^r_d(\triangle)$ by minimizing the thin-plate energy E_2

$$S_j = \arg \min_{s \in S^r_d(\triangle)} \begin{cases} E_2(s), & s(x_i, y_i) = o_{i,j}, i = 1, \cdots, n \\ & s(x,y) \geq 0, (x,y) \in \Omega, \end{cases} \quad (1)$$

where n is the number of observations.
In terms of B-coefficients, we can write

$$s(x,y) = \sum_{i+j+k=d} c^T_{ij} B_{ijk}, \quad \text{if } (x,y) \in T \in \triangle \quad (2)$$

whose coefficient vector $\mathbf{c} = (c^T_{ijk}, i+j+k = d, T \in \triangle)$ of size $N(d+1)(d+2)/2$, where N is the number of triangles in $\triangle$, satisfies the smoothness conditions $H\mathbf{c} = 0$ (Lai and Schumaker 2007). Letting $I\mathbf{c} = \mathbf{o}_j$ be the linear equations for the interpolation conditions in (1) with $\mathbf{o}_j = (o_{1,j}, \cdots, o_{n,j})$, we can rewrite the constrained interpolation problem (1) as

$$\min\{\mathbf{c}^\top E\mathbf{c}, \quad H\mathbf{c} = 0, I\mathbf{c} = \mathbf{o}_j, \mathbf{c} \geq 0\}. \quad (3)$$

where E is the symmetric and nonnegative definite matrix associated with the energy functional, i.e., $\mathbf{c}^\top E\mathbf{c} = E_2(s)$.
To solve (3), we use the Uzawa algorithm (Ciarlet 1989): Start with an initial guess S^0 and initial KKT multiplier vector $\lambda^{(0)} = 10^{-4}$. For $k \geq 1$, we minimize the quadratic function

$$\min_{v \in \mathbb{R}^n} \alpha\mathbf{c}^\top E\mathbf{c} + \|H\mathbf{c}\|_2^2 + \|I\mathbf{c} - \mathbf{o}_j\|_2^2 + (\lambda^{(k)})^\top \mathbf{c} \quad (4)$$

to find $\mathbf{c}^{(k)}$ and update

$$\lambda^{(k+1)} = \max\{\lambda^{(k)} + \rho(\mathbf{c}^{(k)}), 0\}, \quad (5)$$

for $k = 0, 1, 2, \cdots$, where $\rho > 0$ is a step size.

Interpolation of O_2 anomalies

Application to high-resolution model data

The observational data available provides insight into O_2 depletion in the deepwater. However, the information regarding the spatial variability between profiles is limited. Hence, we resorted to results of model simulations (HYCOM; Valentine et al. 2012) assuming that the process based system description leads to meaningful approximation to the actual variability of O_2 anomalies at high resolution. We tuned our interpolation algorithms to match model results (Table 1), and then used this parameterization to interpolate the observational data. Figure 4 gives an example of the reconstruction of the model data.

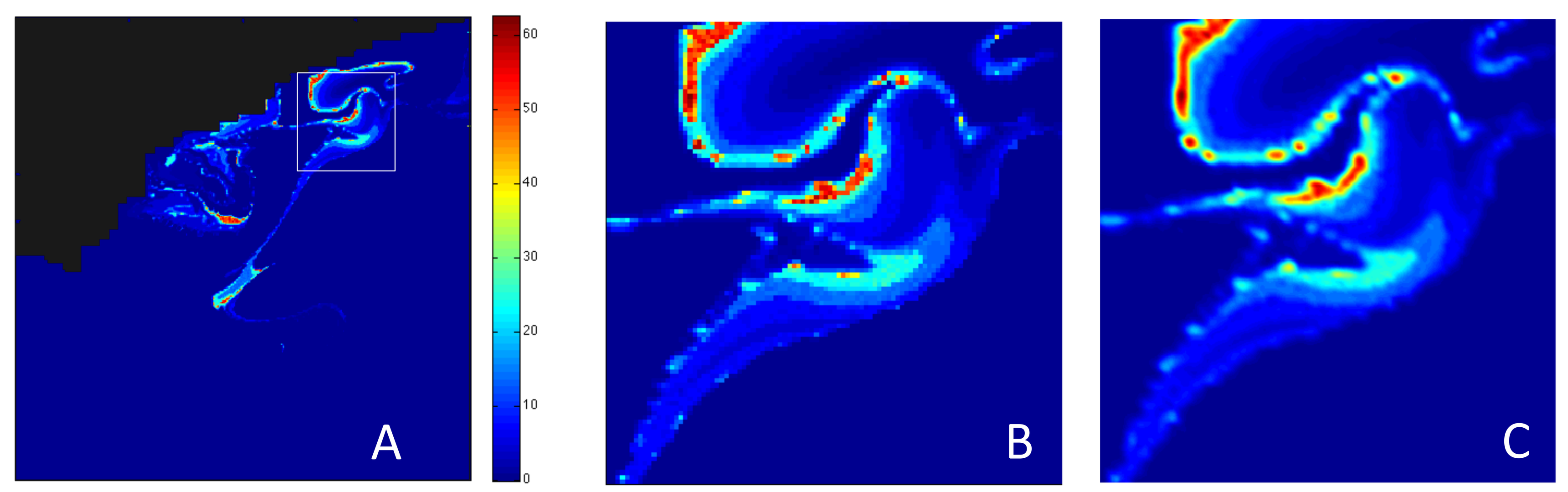

Figure 4: Simulated O_2 anomalies for July 18 in μM (A; Valentine et al. 2012). (B) and (C) show model data and spline reconstruction in the inset ($\alpha = 10^{-8}$).

α	std
10^{-5}	2.7725
10^{-6}	2.5020
10^{-7}	2.4620
10^{-8}	1.7819
10^{-9}	1.7820
10^{-10}	1.7820

Parameterization: a similar pattern of the fit to of the spline interpolation to the simulation data with respect to the smoothing parameter α was found for meshes with different resolution, indicating an optimal α of 10^{-8}.

Table 1: Impact of weighting parameter α on the quality of the spline fit over ~1200 triangles.

Application to the observational data

The bivariate spline implementation shows that the interpolation produces the desired non-negative anomalies and the absence of overshooting (Figure 5). Due to the sparsity of data, the O_2 anomalies appear however smoother than in the high resolution model data (Figure 4).

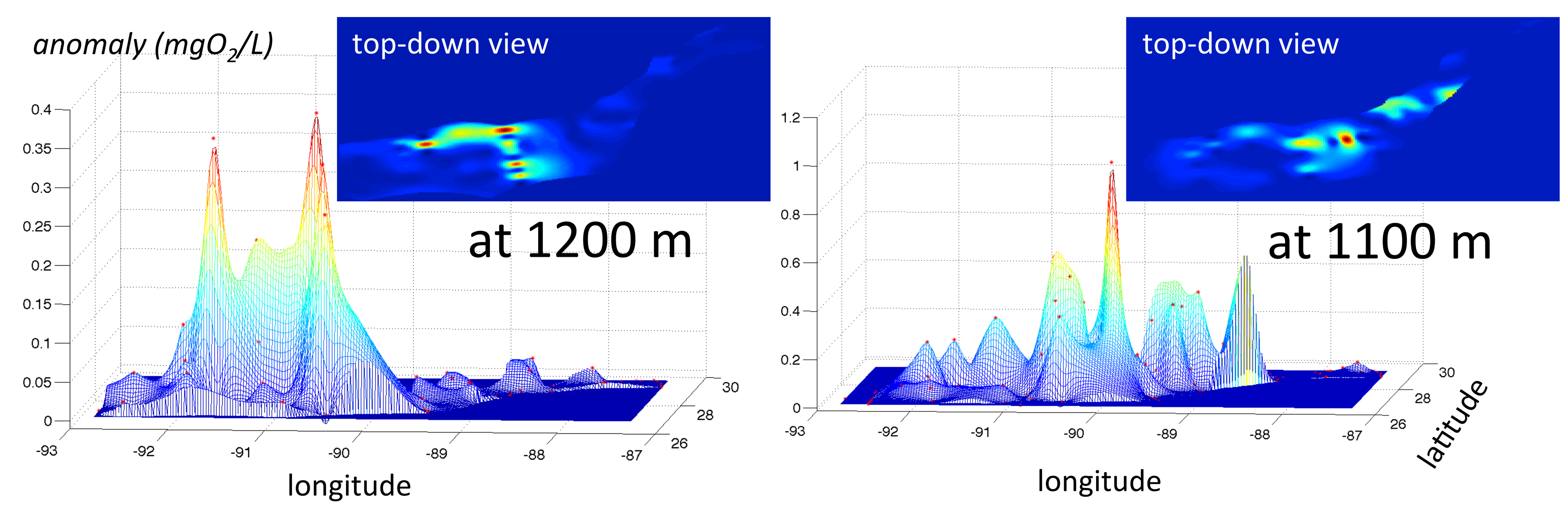

Figure 5: Spatial distribution of O_2 anomalies at 1200 m (left) and 1100 m (right) water depths. Observations (+) are interpolated using bivariate splines. The color coding of top-down views follow the scale given in the respective 3D plot.

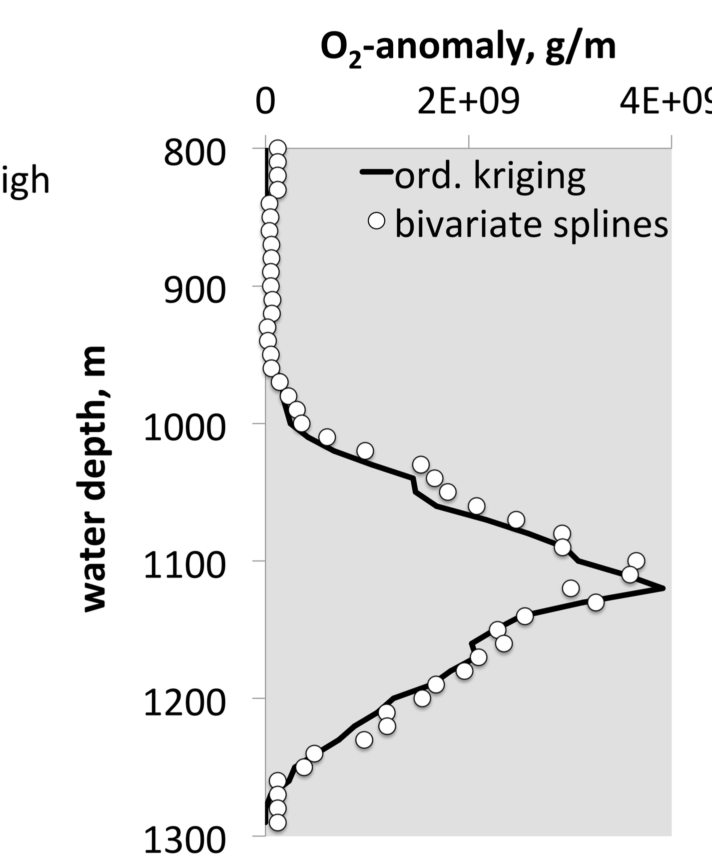

Figure 6: Depth-profile of the estimated O_2 anomaly within the domain (Fig. 3), using bivariate splines & ordinary kriging

Depth-profiles of O_2 anomalies estimated with bivariate splines and ordinary kriging are similar (Fig. 6). However, difference of on the order of 10% exist when comparing the total O_2 anomaly computed using kriging by layer vs. the depth-integrated anomaly at each station.

Findings

1. Our preliminary results show reasonable agreement between the 2 methods employed to quantify O_2 depletion in the deep water.
2. The bivariate splines approach is able to capture the observed patterns, conserves the positivity of the anomalies and does not exhibit over- and under-shooting.
3. Interpolation using kriging by water column layer vs. by depth-integrated O_2 anomalies leads to discrepancies on the order of 10%.
4. Total O_2 drawdown within the model domain is on the order of $1.5x10^{10}$ mol O_2. This is lower than previous estimates (e.g. Kessler et al. 2011), in part due to the more restricted domain boundaries used here.
5. The sparse observational data does not capture the variability seen in model simulations. This challenges the use of any data-fitting technique to quantify total O_2 depletion (and subsequent mass-balance based attribution to processes).

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Acknowledgements

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http://data.nodc.noaa.gov/DeepwaterHorizon/Ship/Pisces/ORR/Cruise_04/