

*JGR Biogeosciences*

Supporting Information for

**Environmental controls, emergent scaling, and predictions of greenhouse gas (GHG) fluxes in coastal salt marshes**

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**Introduction**

The supporting information provides supplementary information about model optimization and performance statistics, presentation of the model in a user-friendly Excel spreadsheet, tables, and figures.

**Text S1: Model optimization and performance statistics**

The Akaike Information Criterion (AIC) (Akaike, 1974) and the Nash-Sutcliffe Efficiency (NSE) were used to select the optimal number of partial least squares (PLS) components in developing the partial least squares regression (PLSR) models. Performance of the PLSR models was assessed by comparing the observed and predicted GHG fluxes. Apart from the model prediction efficiency (NSE), the ratio of root-mean-square error to the standard deviation of observations (RSR) were used to assess model accuracy. NSE = 1.0 refers to a perfect model; NSE < 0 (i.e., negative) indicates that the developed model is a worse predictor than the average of observations of response variable (i.e., flux) as an alternative model. A perfect to very good model usually has an RSR between 0 and 0.50, a good model has an RSR between 0.50 and 0.60, and a satisfactory model has an RSR between 0.60 and 0.70; RSR > 0.70 indicates an unsatisfactory model (Ishtiaq and Abdul-Aziz, 2015). The performance statistics were computed as follows:

 (S1)

 (S2)

 (S3)

where  = the total number of PLS components,  = total number of observations, and  = the ith observed and predicted GHG fluxes (respectively),  is the average of GHG flux observations, and  = standard deviation of the observations.

**Text S2: Presentation of the predictive scaling models in a user-friendly Excel spreadsheet**

A user-friendly, macro-based Excel spreadsheet model named “Coastal Wetland GHG Model (CWGM)” is presented to predict the salt marsh GHG fluxes from instantaneous light (PAR, μmol/m2/s), soil temperature (ST, ºC), and porewater salinity (SS, ppt) data (see *CWGM*, 2018 to download the Excel model). The model equations (Eq. 5-7) were coded in the Excel spreadsheet by using Visual Basic programming language. Further, we expressed the difference between net carbon (CO2) uptake and net carbon (CO2 and CH4) emissions in the salt marshes by a new term, “net atmospheric carbon removal (NACR)”. NACR is related to the net ecosystem carbon balance (NECB) of a wetland as follows: NECB = NACR – net lateral flux. We proposed NACR because the net lateral fluxes between the salt marsh and the bay were not modeled and predicted in this study. A user can estimate the NACR by upscaling the predicted instantaneous fluxes of CO2 and CH4 over the growing period (or any user-defined period) in units of gram carbon (C) per square meter of marsh area (gC/m2). A provision was also included in the Excel model to estimate CH4 emission fluxes based on the IPCC recommended CO2 equivalent global warming potentials (GWP) (Myhre et al., 2013). A “Readme” sheet was provided in the Excel model file to describe model overview, assumptions, inputs/outputs, and detailed operational guidance to the users. Further, an “Example” sheet was included to demonstrate the predictions of GHG fluxes and NACR using a sample dataset. Upon enabling the “macros” in the Excel file, a user needs to input data for PAR, soil temperature, and porewater salinity, and click “RUN” to predict the corresponding GHG fluxes and NACR. The Excel-based model may aid the coastal stakeholders (e.g., reserve managers, restoration practitioners, and policymakers) in tidal wetland monitoring and restorations, economic evaluations of blue carbon, and developing GHG offset protocols.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Site | Statistics |  | NEECO2,uptake  (µmol/m2/s) | PAR  (µmol/m2/s) | ST  (°C) | SS  (ppt) | pH | h  (m) | SM  (%) |
| Sage Lot  Pond | Mean |  | -6.47 | 1464.29 | 18.01 | 29.83 | 6.85 | 0.45 | 64.34 |
| Standard deviation |  | 5.28 | 530.52 | 4.93 | 3.58 | 0.32 | 0.07 | 3.39 |
| Minimum |  | -0.05 | 303.70 | 8.89 | 20.00 | 6.20 | 0.36 | 51.20 |
| Maximum |  | -17.10 | 2080.37 | 26.10 | 36.00 | 7.87 | 0.64 | 68.67 |
| Hamblin  Pond | Mean |  | -10.36 | 1802.87 | 21.01 | 25.88 | 6.49 | 0.46 | 63.78 |
| Standard deviation |  | 4.13 | 180.06 | 0.60 | 5.87 | 0.23 | 0.04 | 2.38 |
| Minimum |  | -5.31 | 1427.45 | 20.06 | 20.00 | 6.05 | 0.42 | 59.47 |
| Maximum |  | -16.52 | 1984.33 | 21.63 | 33.00 | 6.81 | 0.51 | 66.63 |
| Great  Pond | Mean |  | -8.79 | 1049.72 | 22.95 | 29.50 | 6.92 | 0.50 | 63.08 |
| Standard deviation |  | 4.55 | 641.78 | 1.08 | 3.74 | 0.36 | 0.01 | 1.61 |
| Minimum |  | -3.44 | 425.37 | 21.71 | 24.00 | 6.30 | 0.48 | 60.30 |
| Maximum |  | -14.91 | 1987.03 | 24.27 | 34.00 | 7.56 | 0.51 | 65.13 |
| Eel  Pond | Mean |  | -6.73 | 1651.66 | 21.33 | 32.40 | 6.55 | 0.50 | 60.68 |
| Standard deviation |  | 1.40 | 152.25 | 1.56 | 1.52 | 0.16 | 0.00 | 4.46 |
| Minimum |  | -4.38 | 1514.95 | 20.03 | 30.00 | 6.39 | 0.44 | 54.27 |
| Maximum |  | -7.83 | 1906.83 | 24.01 | 34.00 | 6.79 | 0.44 | 65.43 |

Table S1: Marsh-specific summary of the relative linkage datasets for the daytime net uptake fluxes of CO2 and the corresponding environmental drivers for June-October 2013.

Note: NEECO2,uptake, PAR, ST, SS, pH, h, and SM refer to the daytime net uptake fluxes of CO2, photosynthetically active radiation, soil temperature, porewater salinity, pH, well water level, and soil moisture content, respectively. ppt refers to parts per thousand. h represents the water level relative to the base of wells inserted at 40 cm depth from the ground surface of the marshes.

Table S2: Marsh-specific summary of the relative linkage datasets for the net emission fluxes of CH4 and the corresponding environmental drivers for June-October 2013.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Site | Statistics |  | NEECH4,emission  (nmol/m2/s) | PAR  (µmol/m2/s) | ST  (°C) | SS  (ppt) | pH | h  (m) | SM  (%) |
| Sage Lot  Pond | Mean |  | 0.91 | 1359.77 | 19.07 | 28.98 | 6.96 | 0.47 | 63.93 |
| Standard deviation |  | 0.65 | 708.83 | 4.30 | 3.42 | 0.29 | 0.07 | 3.35 |
| Minimum |  | 0.10 | 115.58 | 8.89 | 20.00 | 6.51 | 0.37 | 51.20 |
| Maximum |  | 2.35 | 2080.37 | 26.10 | 34.00 | 7.87 | 0.64 | 68.67 |
| Hamblin  Pond | Mean |  | 2.24 | 1813.95 | 21.70 | 24.20 | 6.60 | 0.47 | 62.66 |
| Standard deviation |  | 0.45 | 235.53 | 2.55 | 4.92 | 0.17 | 0.04 | 5.78 |
| Minimum |  | 1.56 | 1408.70 | 20.06 | 20.00 | 6.38 | 0.43 | 52.50 |
| Maximum |  | 2.83 | 1984.33 | 26.17 | 30.00 | 6.81 | 0.51 | 66.63 |
| Great  Pond | Mean |  | 1.61 | 1155.35 | 23.03 | 30.00 | 6.93 | 0.50 | 63.16 |
| Standard deviation |  | 0.59 | 678.83 | 1.04 | 3.81 | 0.34 | 0.01 | 1.53 |
| Minimum |  | 1.03 | 425.37 | 21.71 | 24.00 | 6.30 | 0.48 | 60.30 |
| Maximum |  | 2.61 | 2000.37 | 24.27 | 34.00 | 7.56 | 0.51 | 65.13 |
| Eel  Pond | Mean |  | 1.18 | 1139.56 | 22.72 | 32.14 | 6.56 | 0.31 | 63.43 |
| Standard deviation |  | 0.44 | 561.53 | 2.64 | 1.68 | 0.14 | 0.16 | 5.38 |
| Minimum |  | 0.69 | 500.37 | 20.03 | 30.00 | 6.39 | 0.13 | 54.27 |
| Maximum |  | 1.74 | 1657.03 | 26.35 | 34.00 | 6.79 | 0.44 | 68.57 |

Note: NEECH4,emission, PAR, ST, SS, pH, h, and SM refer to the net emission fluxes of CH4, photosynthetically active radiation, soil temperature, porewater salinity, pH, well water level, and soil moisture content, respectively. ppt refers to parts per thousand. h represents the water level relative to the base of wells inserted at 40 cm depth from the ground surface of the marshes.

Table S3: Summary of the predictive modeling datasets for GHG fluxes and environmental drivers for May-October 2013 at four salt marshes in Waquoit Bay and adjacent estuaries, MA.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Dataset | Variables | Mean | Standard deviation | Minimum | Maximum |
| Net uptake fluxes of CO2 *Sample size, N = 137* | NEECO2,uptake (µmol/m2/s) | -5.33 | 4.72 | -0.05 | -17.10 |
| PAR (µmol/m2/s) | 1395.53 | 519.73 | 303.7 | 2093.08 |
| ST (oC) | 17.57 | 4.15 | 8.89 | 26.10 |
| SS (ppt) | 30.50 | 4.70 | 10.00 | 40.00 |
| Net emission fluxes of CO2 *Sample size, N = 22* | NEECO2,emission (µmol/m2/s) | 2.46 | 1.13 | 0.92 | 4.25 |
| ST (oC) | 16.31 | 4.89 | 9.63 | 25.26 |
| Net emission fluxes of CH4 *Sample size, N = 107* | NEECH4,emission (nmol/m2/s) | 0.62 | 0.55 | 0.10 | 2.35 |
| ST (oC) | 17.21 | 4.39 | 8.75 | 26.35 |
| SS (ppt) | 31.22 | 3.97 | 20.00 | 40.00 |

Note: NEECO2,uptake, NEECO2,emission, NEECH4,emission, PAR, ST, and SS refer to daytime net uptake fluxes of CO2,net emission fluxes of CO2,net emission fluxes of CH4, photosynthetically active radiation, soil temperature, and porewater salinity, respectively. ppt refers to parts per thousand. The negative sign indicates the net uptake fluxes of CO2.

Table S4: Results of one-way ANOVA to compare the GHG fluxes across the N loading gradient (5-126 kg/ha/year) among the four salt marshes based on the predictive modeling datasets.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Source of variation | Sum of squares | Degrees of freedom | Mean square | F-statistics | F-critical | p-value |
| *Net uptake fluxes of CO2*  *(NEECO2,uptake)* | | | | | | |
| Among marshes | 0.51 | 3 | 0.17 | 0.46 | 2.67 | 0.71 |
| Within marshes | 49.13 | 133 | 0.36 |  |  |  |
| Total | 49.64 | 136 |  |  |  |  |
| *Net emission fluxes of CH4 (NEECH4,emission)* | | | | | | |
| Among marshes | 0.38 | 3 | 0.13 | 0.98 | 2.69 | 0.41 |
| Within marshes | 13.24 | 103 | 0.13 |  |  |  |
| Total | 13.62 | 106 |  |  |  |  |

Note: Significance of difference was evaluated at the 95% level of confidence (p-value < 0.05).

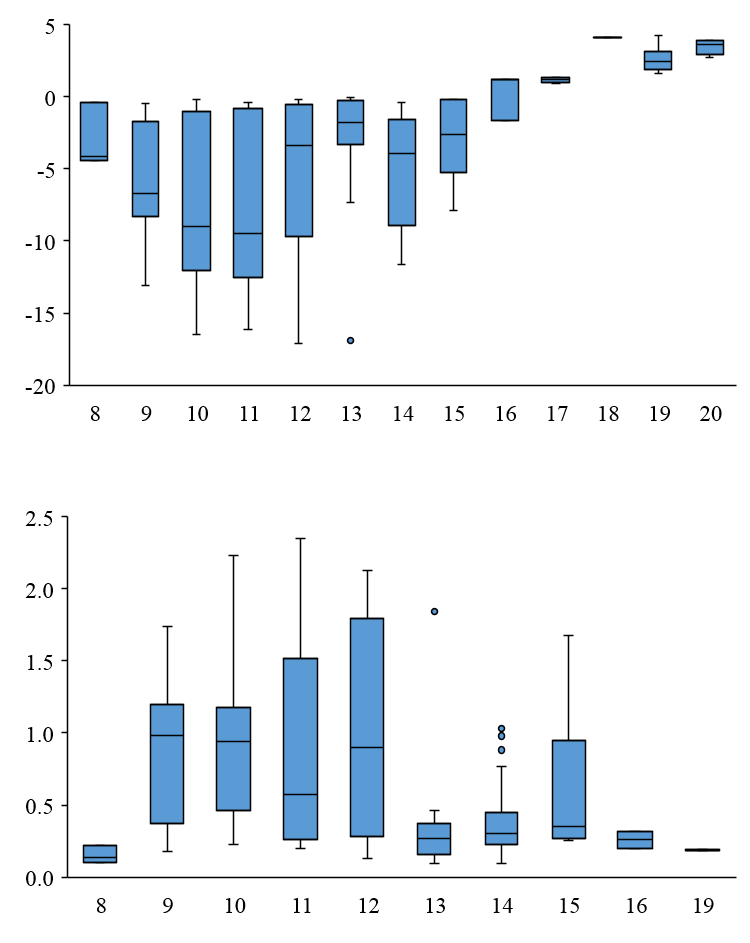
Table S5: Results of one-way ANOVA to compare the GHG fluxes between high and low tide conditions across the four salt marshes based on the predictive modeling datasets.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Source of variation | Sum of squares | Degrees of freedom | Mean square | F-statistics | F-critical | p-value |
| *Net uptake fluxes of CO2 (NEECO2,uptake)* | | | | | | |
| Between tidal conditions | 3.84 | 1 | 3.84 | 11.33 | 3.91 | < 0.001 |
| Within tidal conditions | 45.80 | 135 | 0.34 |  |  |  |
| Total | 49.64 | 136 |  |  |  |  |
| *Net emission fluxes of CH4 (NEECH4,emission)* | | | | | | |
| Between tidal conditions | 2.40 | 1 | 2.40 | 22.47 | 3.93 | < 0.001 |
| Within tidal conditions | 11.22 | 105 | 0.11 |  |  |  |
| Total | 13.62 | 106 |  |  |  |  |

Note: Significance of difference was evaluated at the 95% level of confidence (p-value < 0.05).Table S6: List of 20 downscaled global climate models (GCMs) used to calculate the anticipated changes in GHG fluxes of the salt marshes at Cape Cod, MA.

|  |  |  |
| --- | --- | --- |
| Model Name | Source | Resolution  (Lat. × Lon.) |
| bcc-csm1-1 | Beijing Climate Center, China Meteorological Administration | 2.8˚ × 2.8˚ |
| bcc-csm1-1-m | Beijing Climate Center, China Meteorological Administration | 1.12˚ × 1.12˚ |
| BNU-ESM | College of Global Change and Earth System Science, Beijing Normal University, China | 2.8˚ × 2.8˚ |
| CanESM2 | Canadian Centre for Climate Modeling and Analysis | 2.8˚ × 2.8˚ |
| CCSM4 | National Center of Atmospheric Research, USA | 0.94˚ × 1.25˚ |
| CNRM-CM5 | National Centre of Meteorological Research, France | 1.4˚ × 1.4˚ |
| CSIRO-Mk3-6-0 | Commonwealth Scientific and Industrial Research Organization/Queensland Climate Change Centre of Excellence, Australia | 1.8˚ × 1.8˚ |
| GFDL-ESM2M | NOAA Geophysical Fluid Dynamics Laboratory, USA | 2.0˚ × 2.5˚ |
| GFDL-ESM2G | NOAA Geophysical Fluid Dynamics Laboratory, USA | 2.0˚ × 2.5˚ |
| HadGEM2-ES | Met Office Hadley Center, UK | 1.25˚ × 1.88˚ |
| HadGEM2-CC | Met Office Hadley Center, UK | 1.25˚ × 1.88˚ |
| inmcm4 | Institute for Numerical Mathematics, Russia | 1.5˚ × 2.0˚ |
| IPSL-CM5A-LR | Institut Pierre Simon Laplace, France | 1.8˚ × 3.75˚ |
| IPSL-CM5A-MR | Institut Pierre Simon Laplace, France | 1.25˚ × 2.5˚ |
| IPSL-CM5B-LR | Institut Pierre Simon Laplace, France | 1.8˚ × 2.75˚ |
| MIROC5 | Atmosphere and Ocean Research Institute (The University of Tokyo), National Institute for Environmental Studies,and Japan Agency for Marine-Earth Science and Technology | 1.4˚ × 1.4˚ |
| MIROC-ESM | Japan Agency for Marine-Earth Science and Technology, Atmosphere and Ocean Research Institute (The University of Tokyo), and National Institute for Environmental Studies | 2.8˚ × 2.8˚ |
| MIROC-ESM-CHEM | Japan Agency for Marine-Earth Science and Technology, Atmosphere and Ocean Research Institute (The University of Tokyo), and National Institute for Environmental Studies | 2.8˚ × 2.8˚ |
| MRI-CGCM3 | Meteorological Research Institute, Japan | 1.1˚ × 1.1˚ |
| NorESM1-M | Norwegian Climate Center, Norway | 1.9˚ × 2.5 |

Source: <https://climate.northwestknowledge.net/MACA/GCMs.php>



**(a)**

**CO2 fluxes (µmol/m2/s)**

**(b)**

**Net emission fluxes of CH4 (nmol/m2/s)**

**Hour of the day**

Figure S1: Boxplots of (a) CO2 (NEECO2,uptake andNEECO2,emission) and (b) CH4 (NEECH4,emission) fluxes during May-October 2013 based on the predictive modeling data when binned to the closest diurnal hours in four salt marshes of Waquoit Bay and adjacent estuaries, MA. Negative and positive, respectively, indicate the net uptake and emission fluxes.

**(a)**

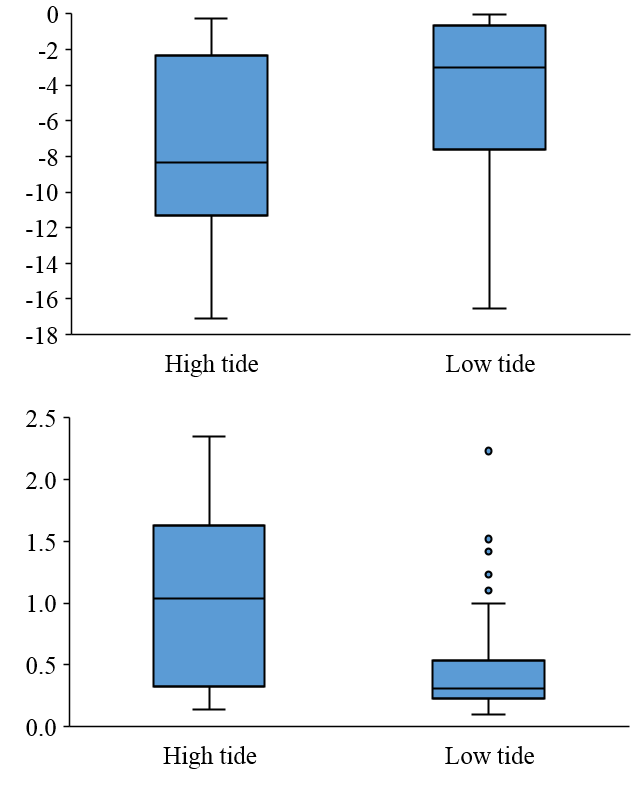
**CO2 fluxes (µmol/m2/s)**

**(b)**

**CH4 fluxes (nmol/m2/s)**

**Julian days**

Figure S2: Temporal plots of measured (a) CO2 (NEECO2,uptake and NEECO2,emission) and (b) CH4 (NEECH4,emission) fluxes during May-October 2013 based on the predictive modeling datasets for four salt marshes at Waquoit Bay and adjacent estuaries, MA. Negative and positive, respectively, indicate the net uptake and emission fluxes.



**(a)**

**Net emission fluxes of CH4 (nmol/m2/s)**

**Net uptake fluxes of CO2 (µmol/m2/s)**

**(b)**

Figure S3: Boxplots of (a) CO2 (NEECO2,uptake) and (b) CH4 (NEECH4,emission) fluxes for high and low tide conditions during May-October 2013 using the predictive modeling datasets for four salt marshes in Waquoit Bay and adjacent estuaries, MA.