

The following supplement accompanies the article

Estimating the effects of seawater intrusion on an estuarine nitrogen cycle by comparative network analysis

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Supplement.

ENA calculations

Reviews of the analyses used in this paper can be found in Fath & Patten (1999), Ulanowicz (2004), and Schramski et al. (2011). We used the *enaR* package to perform our calculations (Lau et al. 2012, Borrett and Lau 2014). This appendix provides only enough information to replicate the results of the accompanying manuscript and is not intended as a comprehensive review of ENA techniques.

Matrix representation

The networks constructed at each site (Fig. 2) were isomorphically represented as two sets of matrices and vectors to facilitate the calculations involved in ENA. The internal N fluxes between nodes for each network were represented in the flow matrix $\mathbf{F} = (f_{ij})$ where i refers to matrix rows (sink compartment) and j refers to matrix columns (source compartment). System inputs and losses to each network were captured in the input vector $\mathbf{z} = (z_i)$ and output vector, $\mathbf{y} = (y_j)$, respectively. The N stored in each pool was represented by the storage vector $\mathbf{x} = (x_i)$. Flow of N in these matrices and vectors was oriented from columns (j) to rows (i).

Flow Analysis

Analyses exist for both the time-backward (input) and time-forward (output) flow orientations that provide different perspectives of the same system (Schramski et al. 2011, Borrett & Freeze 2011). At steady state, the amount of material moving through each network node in the input and output directions is identical. The throughflow of a given node in a network T is calculated as $T_i^{\text{in}} = \sum_{j=1}^n f_{ij} + z_i$ for the input orientation or $T_j^{\text{out}} = \sum_{i=1}^n f_{ij} + y_j$ for the output orientation where n is the number of nodes in the network. At steady state, $T_i^{\text{in}} = T_j^{\text{out}} = T$ for each network node. The work presented in this study utilizes the input-oriented analysis.

Total system throughflow (TST) of a network is the sum of all activity across all nodes and is calculated as $\text{TST} = \sum_{j=1}^n T_j$. TST is distinct from total system throughput, another commonly used network activity metric, in that it incorporates either inputs (z_j) or outputs (y_i), rather than inputs and outputs ($z_j + y_i$), into the throughflow calculation (Fath et al. 2012). TST can be decomposed into boundary, direct, and indirect components. The direct flow intensity matrix \mathbf{G} provides the magnitudes of fluxes traveling from one node to another over a path length of one edge. In the input-oriented direction (denoted by $'$), the direct flow intensity matrix is defined as $\mathbf{G}' = (g'_{ij}) = f_{ij}/T_i$ where T_i is the throughflow in the receiving node. The input-oriented integral flow intensity matrix $\mathbf{N}' = (n'_{ij})$ represents the flow from one network node to another across all path lengths. \mathbf{N}' is the sum of the boundary (\mathbf{G}'^0), direct (\mathbf{G}'^1), and indirect (\mathbf{G}'^m) flow intensity matrices such that

$$\mathbf{N}' = \underbrace{\mathbf{G}'^0}_{\text{boundary}} + \underbrace{\mathbf{G}'^1}_{\text{direct}} + \underbrace{\mathbf{G}'^2 + \dots + \mathbf{G}'^m + \dots}_{\text{indirect}}$$

where m is the path length. The identity $\mathbf{N}' = (\mathbf{G}'^0 - \mathbf{G}'^1)^{-1}$ is used to calculate an exact solution for the integral flow intensity matrix because \mathbf{N}' is a convergent series in steady state networks (Ulanowicz 2004, Borrett et al. 2010).

Environ analysis

Input oriented unit environs e'_{ijk} are calculated by placing elements of the integral flow intensity matrix along the principal diagonal of a square matrix $\delta'_{\ell j}$, then multiplying elements of the direct flow intensity matrix $g'_{i\ell}$ by the resulting matrix such that $e'_{ijk} = g'_{i\ell} \times \delta'_{\ell j}$ where

$$\delta'_{\ell j} = \begin{cases} n'_{ik} & \text{if } \ell = j \\ 0 & \text{if } \ell \neq j \end{cases}$$

The flows in these unit environs are normalized to one. The environ analysis applied in this work utilizes realized input environs \bar{e}'_{ijk} , which are scaled by the observed system boundary flows, rather than normalized to one, as is the case with unit environs (Whipple et al. 2007, Borrett and Freeze, 2011). Realized input environs are calculated by multiplying the input oriented environs by the corresponding network output y_k so that $\bar{e}'_{ijk} = y_k \times e'_{ijk}$. The realized environs produced by these ENA subroutines were used as the inputs for the coupling calculations conducted in this manuscript.

SCOR files

Here, we supply model files for two nitrogen cycling networks, one constructed at an oligohaline site and one constructed at a polyhaline site, in the Cape Fear River Estuary, North Carolina. The models are presented in the format specified by the Scientific Committee on Ocean Research standards (SCOR files, Ulanowicz & Kay 1991), and can be utilized by multiple network analysis packages including enaR for R (Lau et al. 2012, Borrett and Lau 2014) and the DOS based software package NETWRK (Ulanowicz & Kay 1991). The models for the oligohaline and polyhaline sites are presented below, as well as in the downloadable files oligo_cfre.dat and poly_cfre.dat files, respectively. The networks for each site contain eight nodes and can be used in most ecosystem network analyses. The estimation of nitrogen cycling process coupling presented in the manuscript associated with

this supplemental information was conducted using expanded 14 node models. These expanded models were used as an analytical mechanism to maintain the resolution of multiple output fluxes from individual nodes when conducting environ analysis. The 14 node models artificially inflated the TST by converting what were boundary fluxes in the eight-node model to internal flows. Subtracting the sum of the boundary flows from the dummy nodes compensated for this inflation and produces identical TST results to the eight-node model. SCOR files for the fourteen-node versions of each network are available upon request, but were omitted from this publication to avoid confusion. All network analyses outside of this special case within environ analysis should utilize the eight-node networks for each site.

Oligohaline SCOR file:

CFRE OLIGOHALINE SUMMER; HINES&LISA&SONG&TOBIAS&BORRETT;
UNITS=NMOLN/CM3/D;

```
8 2
W-NH4
W-NOx
W-M
W-ON
S-NH4
S-NOx
S-M
S-ON
1 1.05e+01
2 2.76e+01
3 1.00e-03
4 5.40e-01
5 6.83e+02
6 4.19e+00
7 1.00e-02
8 7.11e+03
-1      \IMPORTS
1 1.30e+02
2 1.02e+03
3 3.90e-05
4 1.16e+03
5 1.24e+03
6 1.73e+02
7 0.00e+00
8 7.90e+01
-1      \EXPORTS
1 2.76e+02
```

2 1.01e+03
 3 3.90e-05
 4 1.16e+03
 5 1.08e+03
 6 1.81e+02
 7 3.90e-10
 8 1.08e+02
 -1 \RESPIRATION
 -1 \FLOWS
 3 1 3.09e+00
 4 1 5.20e+00
 5 1 1.37e+02
 1 2 1.70e+00
 6 2 2.15e+00
 1 3 1.90e+00
 2 3 9.80e+00
 4 3 7.40e+00
 7 3 1.19e+02
 3 4 1.60e+01
 8 4 8.50e+02
 1 5 5.50e+00
 6 5 3.89e+01
 7 5 1.47e+02
 8 5 1.50e+02
 2 6 1.41e+01
 5 6 1.44e+02
 3 7 1.19e+02
 5 7 2.13e+02
 6 7 1.09e+02
 8 7 8.20e+01
 4 8 8.54e+02
 7 8 2.57e+02
 -1 -1

Polyhaline SCOR file:

CFRE POLYHALINE SUMMER; HINES&LISA&SONG&TOBIAS&BORRETT,
 UNITS=NMOLN/CM3/D;

8 2
 W-NH4
 W-NOx
 W-M
 W-ON
 S-NH4
 S-NOx
 S-M
 S-ON
 1 2.90e+00
 2 1.51e+01
 3 1.00e-03

4 4.93e+01
5 1.08e+02
6 1.43e+01
7 1.00e-02
8 3.72e+03
-1 \IMPORTS
1 7.25e+01
2 3.811e+02
3 3.90e-05
4 1.2551e+03
5 9.751e+02
6 3.455e+02
7 0.00e+00
8 3.91e+01
-1 \EXPORTS
1 1.324e+02
2 3.809e+02
3 3.90e-05
4 1.2468e+03
5 1.0087e+03
6 2.658e+02
7 3.90e-07
8 3.47e+01
-1 \RESPIRATION
-1 \FLOWS
3 1 3.10e+00
4 1 5.40e+00
5 1 5.53e+01
1 2 7.00e-01
6 2 7.30e+00
1 3 1.70e+00
2 3 5.00e-01
4 3 1.40e+00
7 3 1.192e+02
3 4 5.00e-01
8 4 4.238e+02
1 5 1.50e+00
6 5 1.044e+02
7 5 1.467e+02
8 5 1.00e+02
2 6 7.70e+00
5 6 7.75e+01
3 7 1.192e+02
5 7 1.862e+02
6 7 5.32e+01
8 7 1.596e+02
4 8 4.258e+02
7 8 2.532e+02
-1 -

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