Extreme weather events modulate processing and export of dissolved organic carbon in the Neuse River Estuary, NC

Box model equations and notes

Uploaded to GitHub along with associated Matlab code and data sets:

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The box model was based on a box model developed by Hagy et al., 2000:

Hagy, J.D., Boynton, W.R., Sanford, L.P., 2000. Estimation of Net Physical Transport and Hydraulic Residence Times for a Coastal Plain Estuary Using Box Models. Estuaries 23, 328. https://doi.org/10.2307/1353325

Abbreviations:

R	=	River discharge (averaged over the time period between ModMon sampling runs; obtained from Ft. Barnwell river discharge and scaled to the percent of un-gaged watershed (0.31)).
P (E)	=	Precipitation (evaporation) (obtained from KEWN as the sum of daily precipitation or evaporation) summed over the time period between ModMon sampling runs.
Q_m	=	Surface discharge from the first box.
V_m	=	Surface volume of the first box.
Q_{vm+1}	=	Advective flux from the bottom box to the surface box for the first box.
Q_{m+1}	=	Discharge from the transition box.
V_{m+1}	=	Surface volume of the transition box.
d_{sm+1}	=	Change in salinity between ModMon sampling dates for the surface transition box.
dt	=	Change in time (days) between ModMon sampling dates.
$[Sal]_{m+1}$	=	Surface salinity for the transition box.
$[Sal]'_{m+1}$	=	Bottom salinity for the transition box.
E_{vm+1}	=	Diffusive flux for the transition box.
V'_{m+1}	=	Bottom volume of transition box.
d'_{sm+1}	=	Change in salinity between ModMon sampling dates for the bottom transition box.
Q'_{m+1}	=	Discharge into the bottom transition box.
d_{OC}	=	Change in [OC] between ModMon sampling time points (in days).

$[OC]_R$	=	[OC] in the river end member (Station 0).
$[OC]_m$	=	[OC] in the m box.
p_{OC}	=	The source or sink term for the respective box, as either [DOC] or a_{350}.
P_{sum} (E_{sum})	=	Precipitation (evaporation) summed across boxes upriver from the transition box.
P_m (E_m)	=	Precipitation (evaporation) for the m box.

Notes:

1. See Supplementary information of associated citation (Appendix 4) for a visual depiction of the box model used.
2. The number associated with each abbreviation above (i.e., Q_{m+x}) indicates the box with which the number is associated with (Box 1 – 9) moving down estuary.

Salinity box model:

River Box:

Water balance:

$$R + P = Q_m + E \tag{1}$$

i) Re-arrange equation to solve for Q_m

$$Q_m = R + P - E \tag{2}$$

Note: In the Matlab script, this step is included in the 'Transition box' such that R is the discharge as calculated for the head of the estuary (Station 0), P is summed over the stations above the river box (i.e., if the river box extends until Station 50, P is summed from station 20 to station 50), and E is summed over the same stations as P.

Salt balance: There is no salt balance in the river box.

Transition Box (head of the estuary):

Water balance (surface):

$$Q_m + Q_{\nu m+1} + P = Q_{m+1} + E \tag{3}$$

Water balance (bottom):

$$Q'_{m+1} = Q_{\nu m+1} \tag{4}$$

Salt balance (surface):

$$V_{m+1} * \frac{d_{s_{m+1}}}{dt} = (Q_{\nu m+1} * [Sal]'_{m+1}) - (Q_{m+1} * [Sal]_{m+1}) + E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1}) \tag{5}$$

Salt balance (bottom):

$$V'_{m+1} * \frac{d'_{s_{m+1}}}{dt} = (Q'_{m+1} * [Sal]'_{m+2}) - (Q_{\nu m+1} * [Sal]'_{m+1}) - E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1}) \tag{6}$$

i) Re-arrange the salt balance equations to solve for: $E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1})$

Surface:

$$E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1}) = V_{m+1} * \frac{d_{s_{m+1}}}{dt} + (Q_{m+1} * [Sal]_{m+1}) - (Q_{\nu m+1} * [Sal]'_{m+1}) \tag{7}$$

Bottom:

$$E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1}) = (Q'_{m+1} * [Sal]'_{m+2}) - (Q_{\nu m+1} * [Sal]'_{m+1}) - V'_{m+1} * \frac{d'_{s_{m+1}}}{dt} \tag{8}$$

Re-arrange the surface water balance for Q_{m+1}:

$$Q_{m+1} = Q_m + Q_{\nu m+1} + P - E \tag{9}$$

ii) Substitute Q_{m+1} in the surface salt equation:

$$E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1})$$
$$= V_{m+1} * \frac{d_{s_{m+1}}}{dt} + ((Q_m + Q_{\nu m+1} + P - E) * [Sal]_{m+1}) - (Q_{\nu m+1} * [Sal]'_{m+1}) \quad (10)$$

And substitute $Q_{\nu m+1} = Q'_{m+1}$ in the bottom salt equation:

$$E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1})$$
$$= (Q_{\nu m+1} * [Sal]'_{m+2}) - (Q_{\nu m+1} * [Sal]'_{m+1}) - V'_{m+1} * \frac{d'_{s_{m+1}}}{dt} \quad (11)$$

iii) Then set surface and bottom boxes equal to each other via $E_{\nu m+1}([Sal]'_{m+1} - [Sal]_{m+1})$:

$$V_{m+1} * \frac{d_{s_{m+1}}}{dt} + \left((Q_m + Q_{\nu m+1} + P - E) * [Sal]_{m+1}\right) - (Q_{\nu m+1} * [Sal]'_{m+1})$$
$$= (Q_{\nu m+1} * [Sal]'_{m+2}) - (Q_{\nu m+1} * [Sal]'_{m+1}) - V'_{m+1} * \frac{d'_{s_{m+1}}}{dt} \quad (12)$$

iv) Then expand equation and solve for $Q_{\nu m+1}$, Q'_{m+1}, Q_{m+1}, and $E_{\nu m+1}$:

$$Q_{\nu m+1} = \frac{V'_{m+1} * \frac{d'_{s_{m+1}}}{dt} + V_{m+1} * \frac{d_{s_{m+1}}}{dt} + [Sal]_{m+1}(Q_m + P - E)}{[Sal]_{m+1} - [Sal]'_{m+2}} \quad (13)$$

$$Q'_{m+1} = Q_{\nu m+1} \quad (14)$$

$$Q_{m+1} = Q_m + P - E + \frac{V'_{m+1} * \frac{d'_{s_{m+1}}}{dt} + V_{m+1} * \frac{d_{s_{m+1}}}{dt} + [Sal]_{m+1}(Q_m + P - E)}{[Sal]_{m+1} - [Sal]'_{m+2}} \quad (15)$$

$$E_{\nu m+1} = \frac{V_{m+1} * \frac{d_{s_{m+1}}}{dt} - (Q_{\nu m+1} * [Sal]'_{m+1}) + (Q_{m+1} * [Sal]_{m+1})}{[Sal]'_{m+1} - [Sal]_{m+1}} \quad (16)$$

Estuarine box:

Water balance (surface):

$$Q_{m+1} + Q_{\nu m+2} + P = Q_{m+2} + E \quad (17)$$

Water balance (bottom):

$$Q'_{m+2} = Q'_{m+1} + Q_{\nu m+2} \tag{18}$$

Salt balance (surface):

$$V_{m+2} * \frac{d_{s_{m+2}}}{dt} = (Q_{m+1} * [Sal]_{m+1}) + (Q_{\nu m+2} * [Sal]'_{m+2}) + E_{\nu m+2}([Sal]'_{m+2} - [Sal]_{m+2}) - (Q_{m+2} * [Sal]_{m+2}) \tag{19}$$

Salt balance (bottom):

$$V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} = (Q'_{m+2} * [Sal]'_{m+3}) - (Q'_{m+1} * [Sal]'_{m+2}) - (Q_{\nu m+2} * [Sal]'_{m+2}) - E_{\nu m+2}([Sal]'_{m+2} - [Sal]_{m+2}) \tag{20}$$

i) Re-arrange salt balance equations to solve for $E_{\nu m+2}([Sal]'_{m+2} - [Sal]_{m+2})$:

Surface:

$$E_{\nu m+2}([Sal]'_{m+2} - [Sal]_{m+2}) = V_{m+2} * \frac{d_{s_{m+2}}}{dt} - (Q_{m+1} * [Sal]_{m+1}) - (Q_{\nu m+2} * [Sal]'_{m+2}) + (Q_{m+2} * [Sal]_{m+2}) \tag{21}$$

Bottom:

$$E_{\nu m+2}([Sal]'_{m+2} - [Sal]_{m+2}) = (Q'_{m+2} * [Sal]'_{m+3}) - (Q'_{m+1} * [Sal]'_{m+2}) - (Q_{\nu m+2} * [Sal]'_{m+2}) - V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} \tag{22}$$

Re-arrange the surface water balance to solve for Q_{m+2}:

$$Q_{m+2} = Q_{m+1} + Q_{\nu m+2} + P - E \tag{23}$$

ii) Substitute Q_{m+2} in the surface salinity equation:

$$E_{vm+2}([Sal]'_{m+2} - [Sal]_{m+2})$$

$$= V_{m+2} * \frac{d_{s_{m+2}}}{dt} - (Q_{m+1} * [Sal]_{m+1}) - (Q_{vm+2} * [Sal]'_{m+2}) + ((Q_{m+1} + Q_{vm+2} + P - E) * [Sal]_{m+2}) \tag{24}$$

And substitute Q'_{m+2} in the bottom salinity equation:

$$E_{vm+2}([Sal]'_{m+2} - [Sal]_{m+2})$$

$$= ((Q'_{m+1} + Q_{vm+2}) * [Sal]'_{m+3}) - (Q'_{m+1} * [Sal]'_{m+2}) - (Q_{vm+2} * [Sal]'_{m+2}) - V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} \tag{25}$$

iii) Set surface and bottom salinity equations equal to each other via $E_{vm+2}([Sal]'_{m+2} - [Sal]_{m+2})$:

$$V_{m+2} * \frac{d_{s_{m+2}}}{dt} - (Q_{m+1} * [Sal]_{m+1}) - (Q_{vm+2} * [Sal]'_{m+2}) + ((Q_{m+1} + Q_{vm+2} + P - E) * [Sal]_{m+2}) = ((Q'_{m+1} + Q_{vm+2}) * [Sal]'_{m+3}) - (Q'_{m+1} * [Sal]'_{m+2}) - (Q_{vm+2} * [Sal]'_{m+2}) - V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} \tag{26}$$

iv) Then expand equation and solve for Q_{vm+2}, Q'_{m+2}, Q_{m+2}, and E_{vm+2}:

$$Q_{vm+1} = (V_{m+2} * \frac{d_{s_{m+2}}}{dt} + V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} + Q'_{m+1}([Sal]'_{m+2} - [Sal]'_{m+3}) + Q_{m+1}([Sal]_{m+2} - [Sal]_{m+1}) + \left((P - E) * [Sal]_{m+2}\right))/([Sal]'_{m+3} - [Sal]_{m+2}) \tag{27}$$

$$Q'_{m+2} = Q_{m+1} + (V_{m+2} * \frac{d_{s_{m+2}}}{dt} + V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} + Q'_{m+1}([Sal]'_{m+2} - [Sal]'_{m+3}) + Q_{m+1}([Sal]_{m+2} - [Sal]_{m+1}) + \big((P - E) * [Sal]_{m+2}\big))/([Sal]'_{m+3} - [Sal]_{m+2}) \quad (28)$$

$$Q_{m+2} = Q_{m+1} + P - E + (V_{m+2} * \frac{d_{s_{m+2}}}{dt} + V'_{m+2} * \frac{d'_{s_{m+2}}}{dt} + Q'_{m+1}([Sal]'_{m+2} - [Sal]'_{m+3}) + Q_{m+1}([Sal]_{m+2} - [Sal]_{m+1}) + \big((P - E) * [Sal]_{m+2}\big))/([Sal]'_{m+3} - [Sal]_{m+2}) \quad (29)$$

$$E_{\nu m+2} = \frac{V_{m+2} * \frac{d_{s_{m+2}}}{dt} - (Q_{m+1} * [Sal]_{m+1}) - (Q_{\nu m+2} * [Sal]'_{m+2}) + (Q_{m+2} * [Sal]_{m+2})}{[Sal]'_{m+2} - [Sal]_{m+2}} \quad (30)$$

OC Box Model (as either DOC or a_{350}):

Notes:

1. The salinity box model cannot be used to estimate estuarine discharge when salinity is zero. Therefore, for boxes where no salinity is present (i.e., above the manually defined ‘head of the estuary’) there is no discharge data that can be used in the OC box model and it was assumed the river discharge at Ft. Barnwell was equal to the discharge entering the surface of the transition box.
2. Evaporation and precipitation were accounted for above the head of the estuary by summing precipitation and evaporation not only through time (summed between the ModMon sampling time points) but also summed across stations located above the head of the estuary and added/subtracted within the river discharge (R) term used in the transition box.

3. Evaporation and precipitation were also accounted for in each box by adding/subtracting the precipitation and evaporation value to the discharge value of that specific box.
4. In these equations, a source of p_{oc} is (-) and a sink is (+). In order to follow convention, for the final manuscript, the p_{oc} term was multiplied to (-1) to follow the convention of a source = (+) and a sink = (-).

River Box:

[OC] Balance:

$$V_m * \frac{d_{OC_m}}{dt} = (R * [OC]_R) - ((Q_m + P - E) * [OC]_m) + p_{OC} \tag{31}$$

i) Re-arrange to solve for p_{OC} term:

$$p_{OC} = V_m * \frac{d_{OC_m}}{dt} - (R * [OC]_R) + ((Q_m + P - E) * [OC]_m) \tag{32}$$

Transition box (head of estuary):

Surface [OC] balance:

$$\begin{aligned} V_{m+1} * \frac{d_{OC_{m+1}}}{dt} \\ &= \big((R + P_{sum} - E_{sum}) * [OC]_R\big) + (Q_{\nu m+1} * [OC]'_{m+1}) \\ &+ E_{\nu m+1}([OC]'_{m+1} - [OC]_{m+1}) - ((Q_{m+1} + P_{m+1} - E_{m+1})) + p_{OC} \end{aligned} \tag{33}$$

i) Solve equation of p_{OC}:

$$\begin{aligned} p_{OC} = V_{m+1} * \frac{d_{OC_{m+1}}}{dt} - \big((R + P_{sum} - E_{sum}) * [OC]_R\big) - (Q_{\nu m+1} * [OC]'_{m+1}) \\ - E_{\nu m+1}([OC]'_{m+1} - [OC]_{m+1}) + ((Q_{m+1} + P_{m+1} - E_{m+1})) \end{aligned} \tag{34}$$

Bottom [OC] balance:

$$V'_{m+1} * \frac{d'_{OC_{m+1}}}{dt} = (Q'_{m+1} * [OC]'_{m+2}) - (Q_{\nu m+1} * [OC]'_{m+1}) - E_{\nu m+1}([OC]'_{m+1} - [OC]_{m+1}) + p_{OC} \quad (35)$$

i) Solve equation of p_{oc}:

$$p_{OC} = V'_{m+1} * \frac{d'_{OC_{m+1}}}{dt} - (Q'_{m+1} * [OC]'_{m+2}) + (Q_{\nu m+1} * [OC]'_{m+1}) + E_{\nu m+1}([OC]'_{m+1} - [OC]_{m+1}) \quad (36)$$

Estuarine box:

Surface [OC] balance:

$$V_{m+2} * \frac{d_{OC_{m+2}}}{dt} = (Q_{m+1} * [OC]_{m+1}) + (Q_{\nu m+2} * [OC]'_{m+2}) + E_{\nu m+2}([OC]'_{m+2} - [OC]_{m+2}) - ((Q_{m+2} + P_m - E_m) * [OC]_{m+2}) + p_{OC} \quad (37)$$

i) Solve equation of p_{OC}:

$$p_{OC} = V_{m+2} * \frac{d_{OC_{m+2}}}{dt} - (Q_{m+1} * [OC]_{m+1}) - (Q_{\nu m+2} * [OC]'_{m+2}) - E_{\nu m+2}([OC]'_{m+2} - [OC]_{m+2}) + ((Q_{m+2} + P_m - E_m) * [OC]_{m+2}) \quad (38)$$

Bottom [OC] balance:

$$V'_{m+2} * \frac{d'_{OC_{m+2}}}{dt} = (Q'_{m+2} * [OC]'_{m+3}) - (Q'_{m+1} * [OC]'_{m+2}) - (Q_{\nu m+2} * [OC]'_{m+2}) - E_{\nu m+2}([OC]'_{m+2} - [OC]_{m+2}) + p_{OC} \quad (39)$$

i) Solve equation for p_{OC}:

$$p_{OC} = V'_{m+2} * \frac{d'_{OC_{m+2}}}{dt} - (Q'_{m+2} * [OC]'_{m+3}) + (Q'_{m+1} * [OC]'_{m+2}) + (Q_{\nu m+2} * [OC]'_{m+2}) + E_{\nu m+2}([OC]'_{m+2} - [OC]_{m+2}) \tag{40}$$