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Source-to-sink pathways of dissolved organic carbon in the river–estuary–ocean continuum: a modeling investigation

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Text S1. DOC cycle module

The equations for the conservation of dissolved carbon in all pools are provided as follows. The labile DOC (R_1) is affected by bacteria mortality and uptake, phytoplankton mortality, and zooplankton excretion and mortality:

$$\frac{\partial R_1}{\partial t} = f^t r_{mort} B_c - min(1, \frac{G_{env}}{G_{sub}}) n_1 R_1 + (1 - min(\frac{qp_{min}}{q_{P:C}}, \frac{qn_{min}}{q_{N:C}}, 1.0)) f_{lysis} P_c + q_{R_1} q_{dis} (1.0 - a_e) q_{exc} r_{ass} f^t \frac{F_c^{total}}{F_c^{total} + h_f} Z_c + q_{R_1} q_{dis} ((1 - eO_2) r_{mortox} + r_{mort}) Z_c$$

where f^t is a temperature–dependent growth function (Blackford et al., 2004). r_{mort} represents the basal mortality rate, and B_c is the bacterial carbon. The bacterial uptake depends on the magnitude of both maximum potential uptake G_{env} and substrate availability G_{sub}. n_1 signifies the fraction of R1 available to bacteria. Within the phytoplankton lysis term, qp_{min} and qn_{min} represent the minimal P/C and N/C ratio, respectively. $q_{P:C}$ and $q_{N:C}$ are the instantaneously calculated P/C and N/C cellular ratios, respectively. f_{lysis} is the nutrient-stress lysis rate which occurs proportionally to the current biomass. P_c is phytoplankton biomass. In the last two terms, q_{R_1} is the labile fraction of produced dissolved organic carbon. q_{dis} is the dissolved fraction of excreted/dying matter. a_e is the assimilation efficiency, q_{exc} is the fraction of unassimilated prey that is excreted. r_{ass} is maximal assimilation rate at reference temperature. F_c^{total} signifies the carbon of total food available. h_f is the food concentration where uptake is 0.5. Z_c is the biomass of zooplankton. eO_2 is an oxygen limitation factor, r_{mortox} represents the mortality rate at low oxygen concentrations.

The semi-labile DOC (R_2) is affected by bacteria release and uptake, phytoplankton excretion:

$$\frac{\partial R_2}{\partial t} = max\left[0, \max\left(1 - \frac{q_{P:C}}{p^{opt}}, 1 - \frac{q_{N:C}}{n^{opt}}\right)\right] B_c \nu - \min(1, \frac{G_{env}}{G_{sub}}) n_2 R_2 + (p_{ex} + (1 - iNI)(1 - p_{ex})) f_{phosyn} P_c$$

where p^{opt} and n^{opt} are maximum phosphorus to carbon ratio and maximum nitrogen to carbon ratio. ν is the characteristic time-scale of the process (supposed to be 1 d). n_2 denotes the fraction of R_2 available to bacteria. p_{ex} signifies the portion of primary production released as activity-dependent excretion. iNI is co-limitation of inorganic nitrogen and phosphorus (Droop, 1974). f_{phosyn} represents the gross photosynthetic activity rate.

The semi-refractory DOC (R_3) is influenced by bacteria excretion and uptake:

$$\frac{\partial R_3}{\partial t} = q_{R_3}(1 - r_{resp}O_{rel} - r_{respox}(1 - O_{rel}))min(1,\frac{G_{env}}{G_{sub}}) - min(1,\frac{G_{env}}{G_{sub}})n_3R_3$$

It is assumed that the proportion of recalcitrant carbon released in the form of semi-refractory material is determined by a factor q_{R_3} related to the metabolic cost of uptake activity. r_{resp} and r_{respox} represent the efficiency of the respired fraction of carbon uptake under high and low oxygen conditions, respectively. O_{rel} is relative oxygen saturation. n_3 is fraction of R3 available to bacteria.

The T_1 includes river input, photo-oxidation, bacterial uptake, and flocculation. The photo-oxidation process is only considered in the surface layer.

$$\frac{\partial T_1}{\partial t} = \left.\frac{\partial T_1}{\partial t}\right|_{river} - (1 + q_a)r_{phooxi}\frac{Iq_{scaling}}{I_{ref}}T_1 - min\left(1,\frac{G_{env}}{G_{sub}}\right)n_{T1}T_1 - r_{floc}e^{\frac{-(ln(Sal)-i_{flocmax})^2}{2i_{PAR}{}^2}}T_1{}^2$$

where q_a is fraction of tDOC aging due to photo-oxidation, r_{phooxi} is reference surface photo-oxidation rate. I and I_{ref} are instantaneous irradiance and reference surface photo-oxidation rate, respectively. $q_{scaling}$ is the scaling factor for incoming radiation activating photochemical reaction. n_{T1} is fraction of T_1 available to bacteria. r_{floc} is the maximum flocculation rate, $i_{flocmax}$ represents the logarithm of salinity at the point of maximum flocculation. i_{PAR} is the salinity function parameter.

The T_2 includes river input, transformation from T_1, and bacterial uptake.

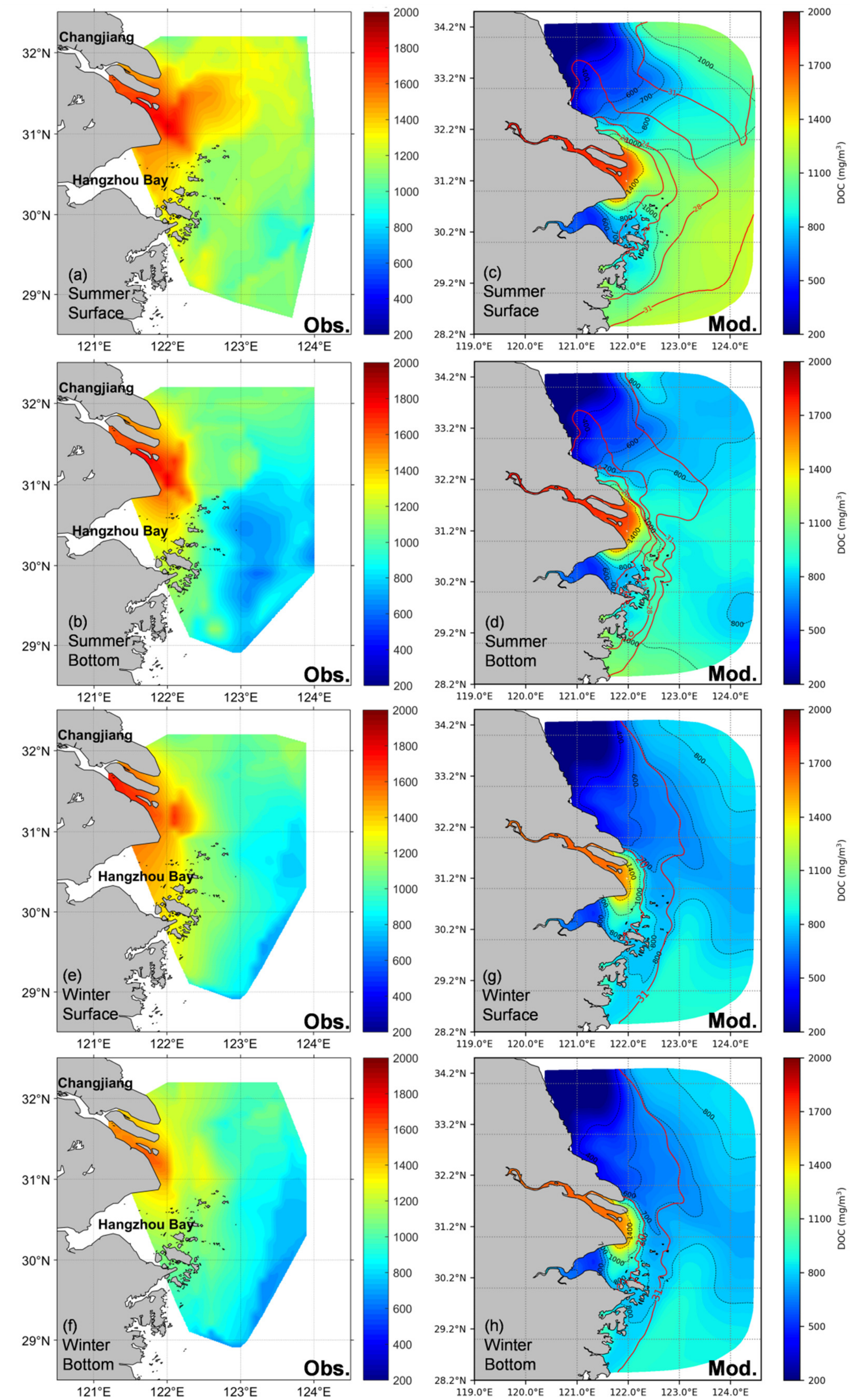
$$\frac{\partial T_2}{\partial t} = \left.\frac{\partial T_2}{\partial t}\right|_{river} + q_{T_1T_2}(1 + q_a)r_{phooxi}\frac{Iq_{scaling}}{I_{ref}}T_1 - min\left(1,\frac{G_{env}}{G_{sub}}\right)n_{T2}T_2$$

where $q_{T_1T_2}$ is photo-oxidated fraction of T_1 going into T_2. n_{T2} is fraction of T_2 available to bacteria. The key configuration of parameters related to DOC cycling are listed in Table S1.

Table S1. Key parameters configuration related to DOC cycling in the FVCOM-ERSEM model.

Notation	Description	Value	Unit
Bacteria		B1	
rR2	Availability of R2	0.04	-
rR3	Availability of R3	0.002	-
rTD1	Availability of T1 pool1	0.00282	-
rTD2	Availability of T1 pool2	0.000501	-
rTD3	Availability of T1 pool3	0.00022	-
rTD4	Availability of T2 pool1	0.00848	-

rTD5	Availability of T2 pool2	0.001508				-
rTD6	Availability of T2 pool3	0.000661				-
Phytoplankton	Diatoms (P1), nanophytoplankton (P2), picoplankton (P3), and microphytoplankton (P4)	P1	P2	P3	P4	
sum	Assimilation rate at 10 °C	0.825	0.975	1.2	0.675	1 d-1
Zooplankton	Mesozooplankton(Z4), microzooplankton (Z5), heterotrophic flagellates (Z6)	Z4	Z5	Z6		
sum	Assimilation rate at 10 °C	1	1.75	2.1		1 d-1
T1	Photolabile tDOC(T1_30d), aging T1_30d(T1_8y), aging T1_8y (T1_70y)	T1_30d	T1_8y	T1_70y		
photoaging	Fraction of tDOC aging	0.5	0.025	0		-
bioaging	Aging due to microbial degradation	0.5	0.025	0		
surf_phyref	Reference photooxidation rate	0.05175	0.0092	0.00404		1 d-1
floc	Maximal flocculation rate	0.000002	0.000002	0.000002		d-1 mg-1 C
phyt	Photo-oxidated fraction of T1 into T2	0.24	0.24	0.24		-
T2	Non-photolabile tDOC(T2_30d), aging T2_30d(T2_8y), aging T2_8y (T2_70y)	T2_30d	T2_8y	T1_70y		
bioaging	Aging due to microbial degradation	0.1	0.005	0		-



Changjiang
Hangzhou Bay
(a) Summer Surface
Obs.
(c) Summer Surface
Mod.
(b) Summer Bottom
(d) Summer Bottom
(e) Winter Surface
(g) Winter Surface
(f) Winter Bottom
(h) Winter Bottom
DOC (mg/m^3)
121°E
122°E
123°E
124°E
29°N
30°N
31°N
32°N
119.0°E
120.0°E
121.0°E
122.0°E
123.0°E
124.0°E
28.2°N
29.2°N
30.2°N
31.2°N
32.2°N
33.2°N
34.2°N

Figure S1. The average distribution of DOC concentration in both the surface and bottom layers during summer and winter, comparing observational data (left column) with model data (right column).

References

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