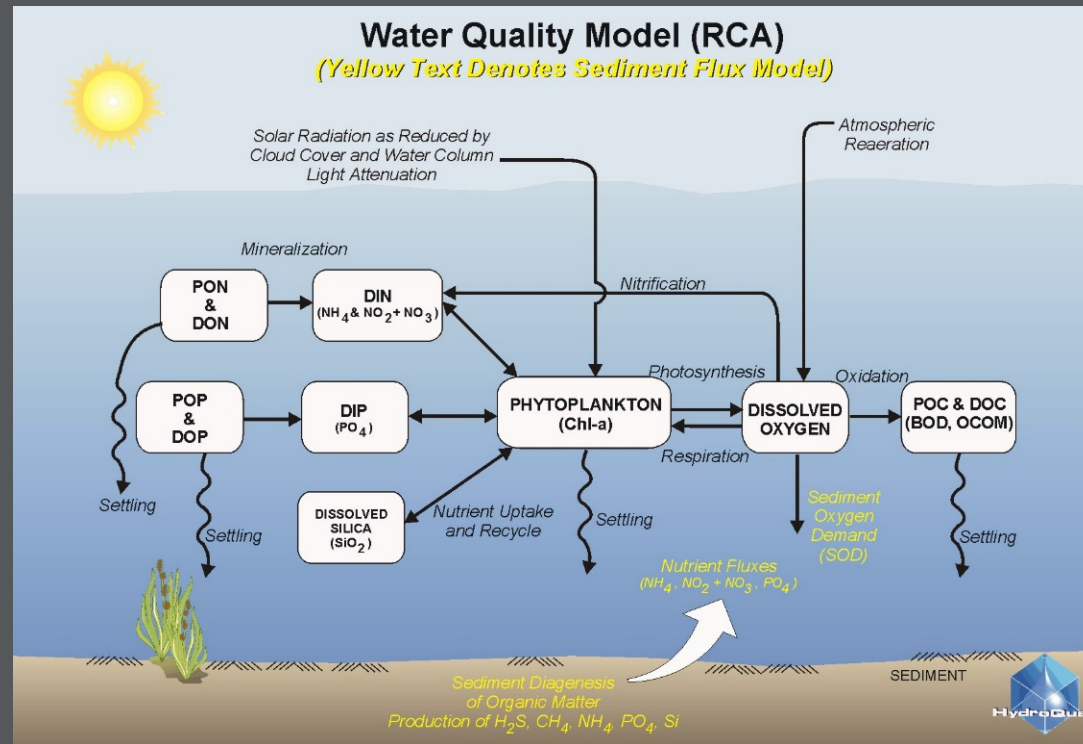
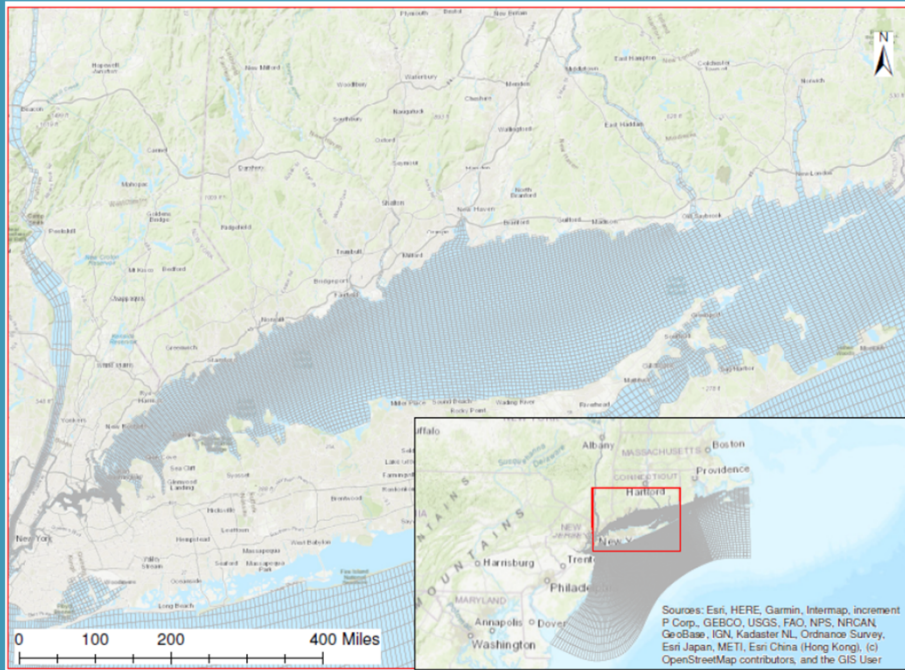




LIS ROMS-RCA MODEL

Water Quality Model Theory



01 **LIS MODEL OVERVIEW**

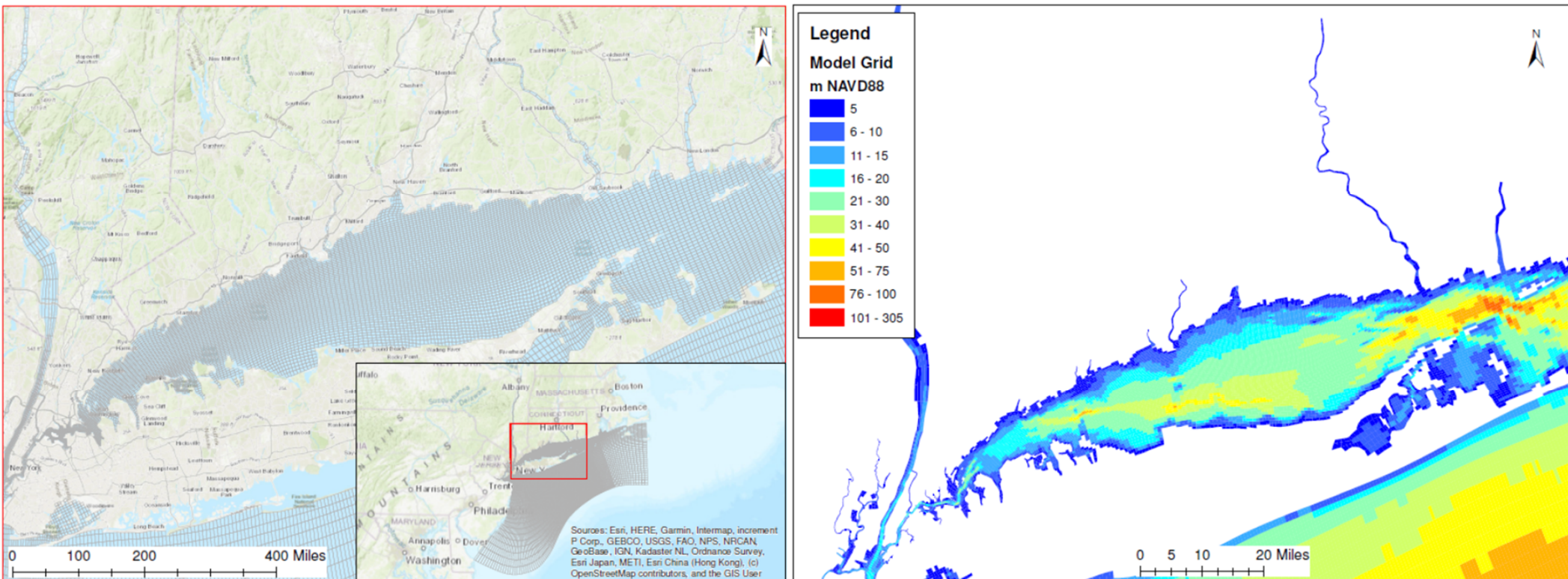
02 **ROMS HYDRODYNAMIC MODEL**

03 **RCA WATER QUALITY MODEL**

04 **ROMS-RCA DETAILS**

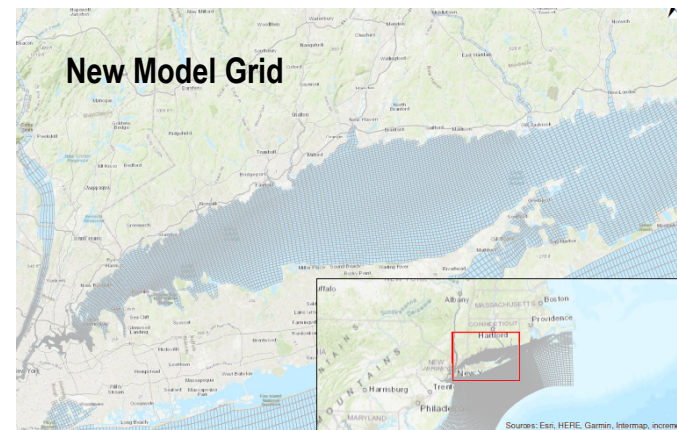
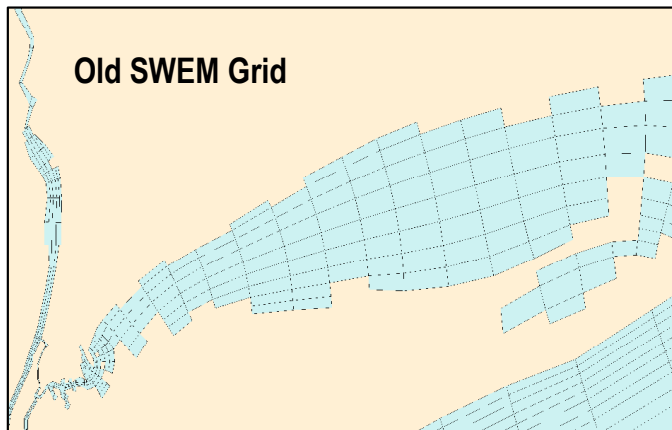
LIS ROMS-RCA MODEL OVERVIEW

- Funded jointly by NYCDEP & EPA (started in 8/2020, ending 8/2026)
 - Update LIS models, 2 embayment models, model GUI, living resources model demonstration



PRIOR LIS SWEM MODEL (LATE 90s/EARLY 00s)

- Coarse spatial grid LIS model developed & used to support 2000 TMDL
 - ECOM hydrodynamic model & RCA water quality model
 - Grid resolution driven by computing resources at the time
- Independent review of SWEM identified a number of concerns
 - Primary concern was that ECOM vertical mixing needed to be reduced in RCA to reproduce DO data
 - Other concerns related to algal primary production & respiration, SOD & nutrient fluxes



LIS ROMS-RCA MODEL OVERVIEW

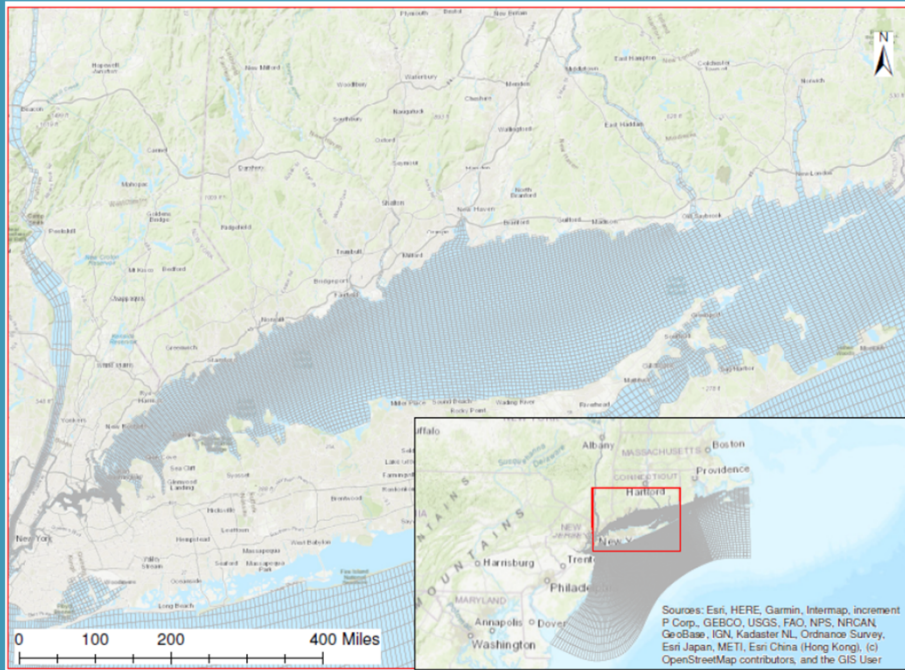
- Model calibration – 2005-2014
- Model validation – 2003-2004, 2015-2018
- Model post-audit – 2019-2022

- Three management scenarios
 - Pre-development
 - Post-development
 - Nutrient Bioextraction

- Final documentation to date at:
 - <https://lispartnership.org/research-monitoring/scientific-modeling/systemwide-regional-modeling/>

- Model/GUI training (June)

Scenario Name	Objective	Assumptions/Description	Comments
Pre-development condition	Establish a baseline nutrient load that can be compared to other scenarios.	Assume pre-development conditions (i.e., pastoral, forested, non-agricultural landscape; remove all WWTPs, CSOs, SW; reduce river/GW sources & ocean BCs). Assume climate as is.	Climate has changed from pre-development conditions. Does not assess changes in hydrology (e.g., East River deepening), and habitats (loss of wetlands) on nutrient processing and flux.
Post-development condition	Assess how implemented and planned actions will affect nutrient loads.	Model effects of constructed and planned commitments (e.g., POTW upgrades, LINAP reductions, CT Second Generation Strategy, CSOs, remaining, additional BMPs, air depositions projections)	Can include projected population increases that would mitigate future improvements. Need list of future commitments to be included.
Bioextraction/ Sugar Kelp modeling	Assess the potential for sugar kelp to be used develop LIS nutrient uptake strategies.	Model will be developed for open waters in Western LIS. Assume post-development conditions.	This scenario provides an opportunity to apply the biodynamic Sugar Kelp model being developed for the Integrated Modeling Framework.



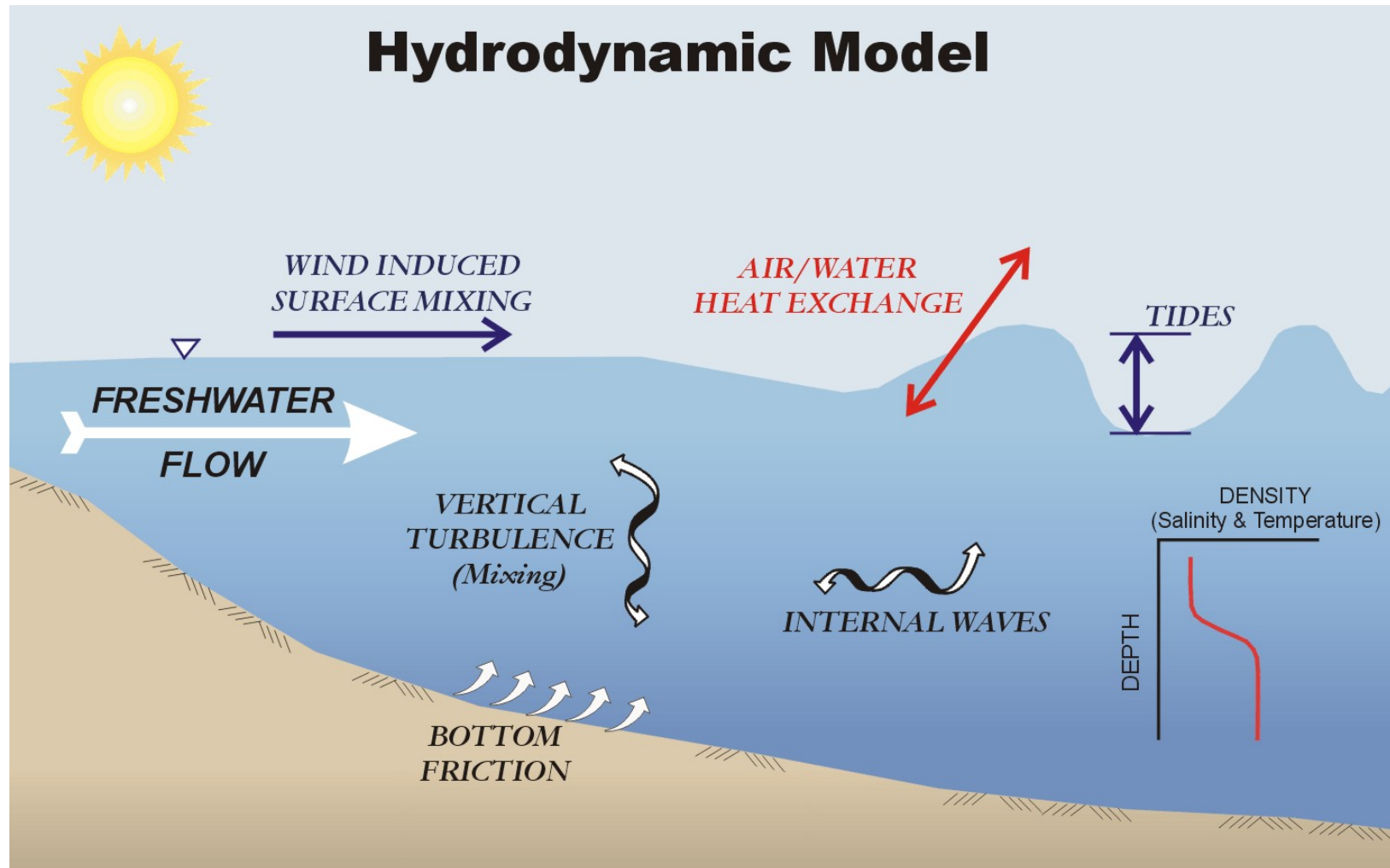
01 LIS MODEL OVERVIEW

02 ROMS HYDRODYNAMIC MODEL

03 RCA WATER QUALITY MODEL

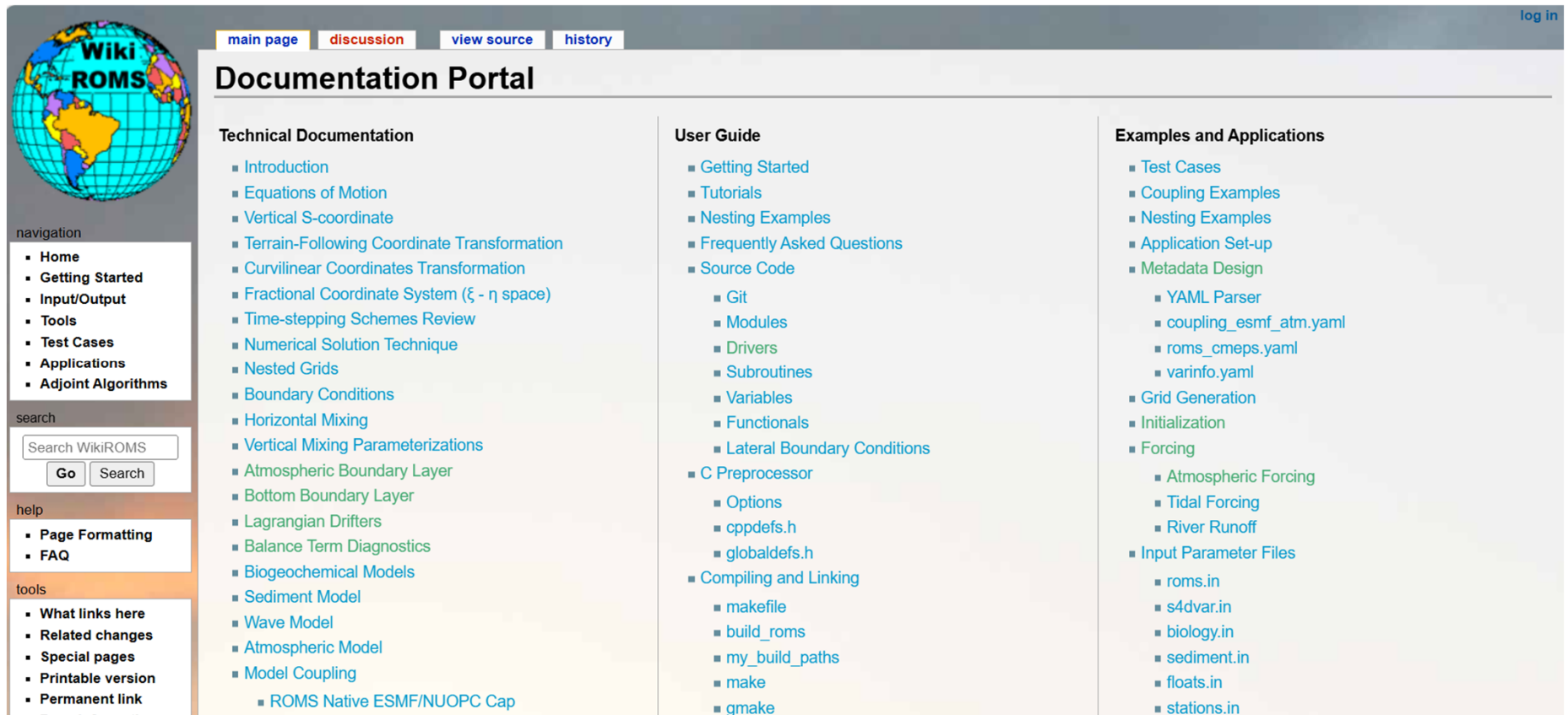
04 ROMS-RCA DETAILS

ROMS HYDRODYNAMIC MODEL



ROMS HYDRODYNAMIC MODEL

- <https://www.myroms.org/>



The screenshot displays the WikiROMS Documentation Portal. At the top, there is a navigation bar with links for 'main page', 'discussion', 'view source', and 'history', along with a 'log in' link in the top right corner. The main content area is titled 'Documentation Portal' and is divided into three columns: 'Technical Documentation', 'User Guide', and 'Examples and Applications'. The left sidebar contains a 'WikiROMS' logo, a 'navigation' menu with links like 'Home', 'Getting Started', 'Input/Output', 'Tools', 'Test Cases', 'Applications', and 'Adjoint Algorithms', a 'search' box, a 'help' section with 'Page Formatting' and 'FAQ', and a 'tools' section with 'What links here', 'Related changes', 'Special pages', 'Printable version', and 'Permanent link'. The 'Technical Documentation' column lists topics such as 'Introduction', 'Equations of Motion', 'Vertical S-coordinate', 'Terrain-Following Coordinate Transformation', 'Curvilinear Coordinates Transformation', 'Fractional Coordinate System (ξ - η space)', 'Time-stepping Schemes Review', 'Numerical Solution Technique', 'Nested Grids', 'Boundary Conditions', 'Horizontal Mixing', 'Vertical Mixing Parameterizations', 'Atmospheric Boundary Layer', 'Bottom Boundary Layer', 'Lagrangian Drifters', 'Balance Term Diagnostics', 'Biogeochemical Models', 'Sediment Model', 'Wave Model', 'Atmospheric Model', and 'Model Coupling'. The 'User Guide' column lists 'Getting Started', 'Tutorials', 'Nesting Examples', 'Frequently Asked Questions', 'Source Code' (with sub-links for 'Git', 'Modules', 'Drivers', 'Subroutines', 'Variables', 'Functionals', and 'Lateral Boundary Conditions'), 'C Preprocessor' (with sub-links for 'Options', 'cppdefs.h', and 'globaldefs.h'), and 'Compiling and Linking' (with sub-links for 'makefile', 'build_roms', 'my_build_paths', 'make', and 'gmake'). The 'Examples and Applications' column lists 'Test Cases', 'Coupling Examples', 'Nesting Examples', 'Application Set-up', 'Metadata Design' (with sub-links for 'YAML Parser', 'coupling_esmf_atm.yaml', 'roms_cmeps.yaml', and 'varinfo.yaml'), 'Grid Generation', 'Initialization', 'Forcing' (with sub-links for 'Atmospheric Forcing', 'Tidal Forcing', and 'River Runoff'), and 'Input Parameter Files' (with sub-links for 'roms.in', 's4dvar.in', 'biology.in', 'sediment.in', 'floats.in', and 'stations.in').

WikiROMS

main page discussion view source history

Documentation Portal

Technical Documentation

- Introduction
- Equations of Motion
- Vertical S-coordinate
- Terrain-Following Coordinate Transformation
- Curvilinear Coordinates Transformation
- Fractional Coordinate System (ξ - η space)
- Time-stepping Schemes Review
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- Balance Term Diagnostics
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- Sediment Model
- Wave Model
- Atmospheric Model
- Model Coupling
 - ROMS Native ESMF/NUOPC Cap

User Guide

- Getting Started
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 - globaldefs.h
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 - gmake

Examples and Applications

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navigation

- Home
- Getting Started
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- Adjoint Algorithms

search

Search WikiROMS

Go Search

help

- Page Formatting
- FAQ

tools

- What links here
- Related changes
- Special pages
- Printable version
- Permanent link

MODEL INPUTS

- Coastline used to develop model grid (channels important considerations)
- Bathymetry used to assign water depth to model cells
- Model grid is orthogonal & used 10 vertical layers

- Rivers (freshwater inputs)
- WWTPs, CSOs, SW
- Groundwater

- Meteorological (wind speed/direction, air temperature, solar radiation, relative humidity)

- Coefficients (bottom roughness, horizontal/vertical dispersive mixing)

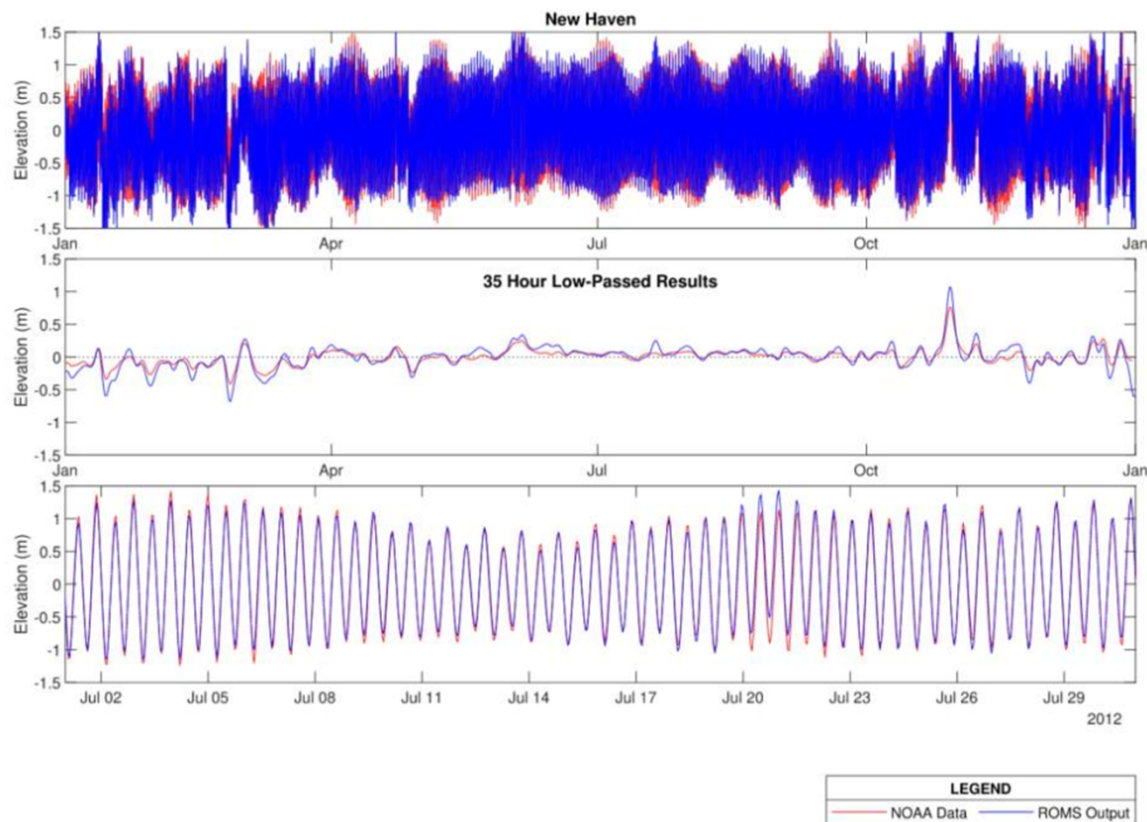
MODEL CALIBRATION/VALIDATION

- Model output compared to data for:

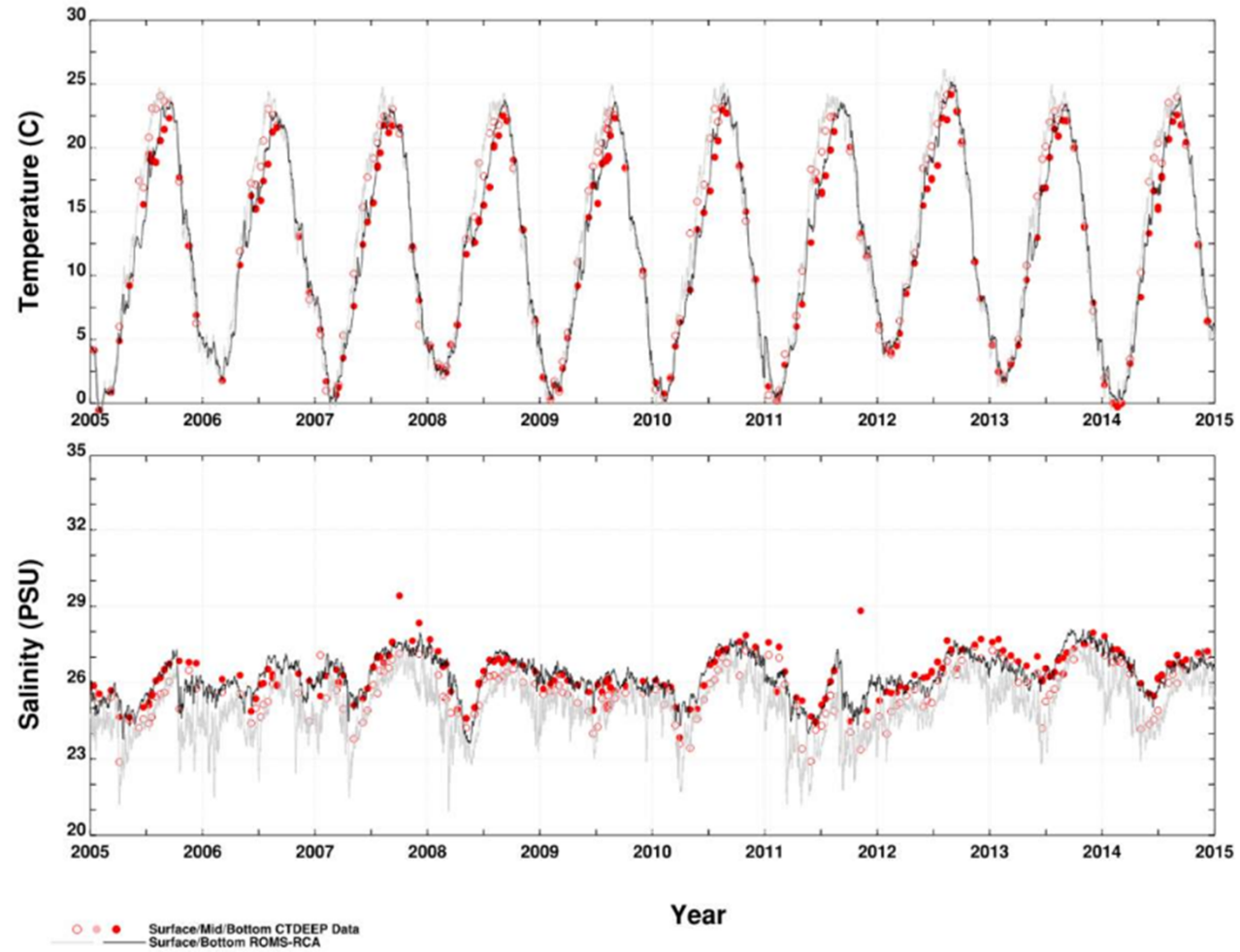
- Water surface elevation
- Temperature
- Salinity
- Current speeds
- East River fluxes

- Datasets used:

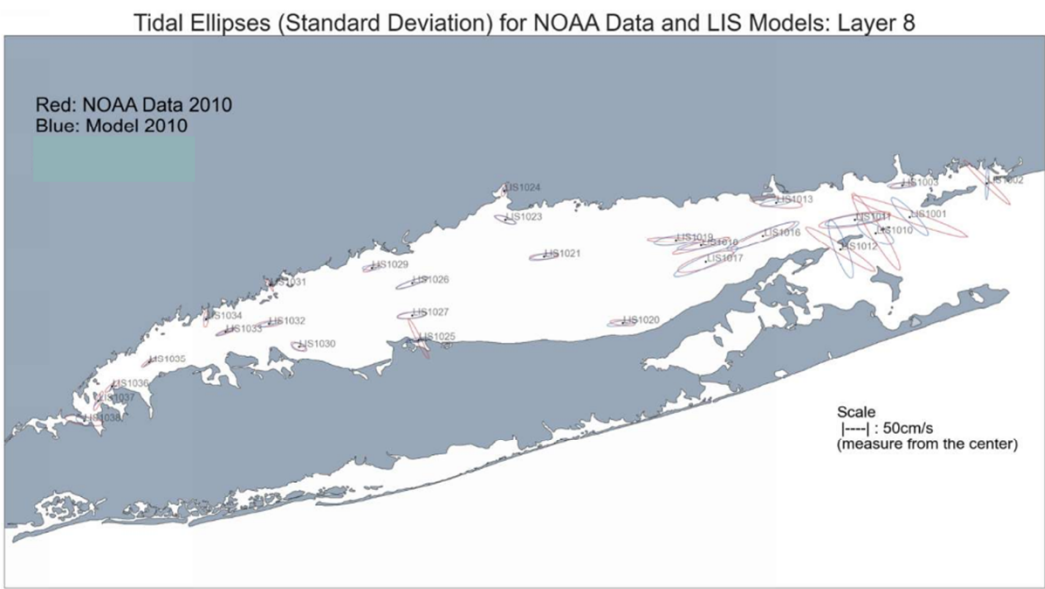
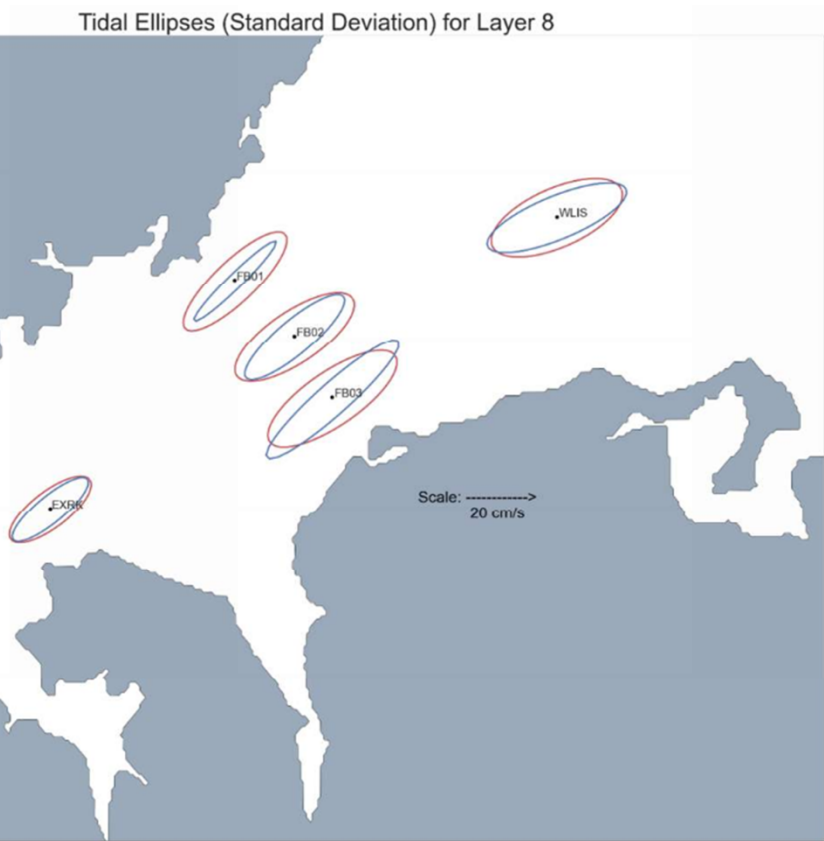
- CTDEEP
- NYCDEP Harbor Survey
- IEC
- NJHDG
- LISICOS
- NOAA



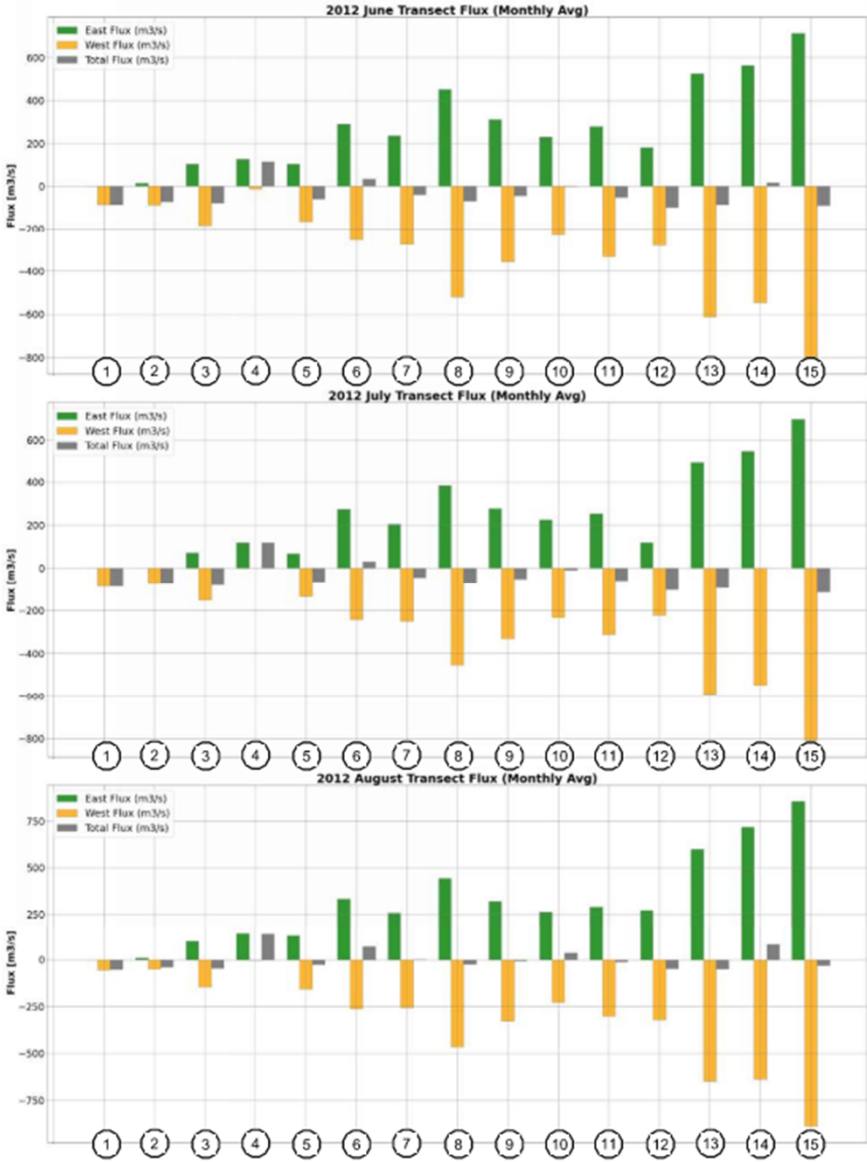
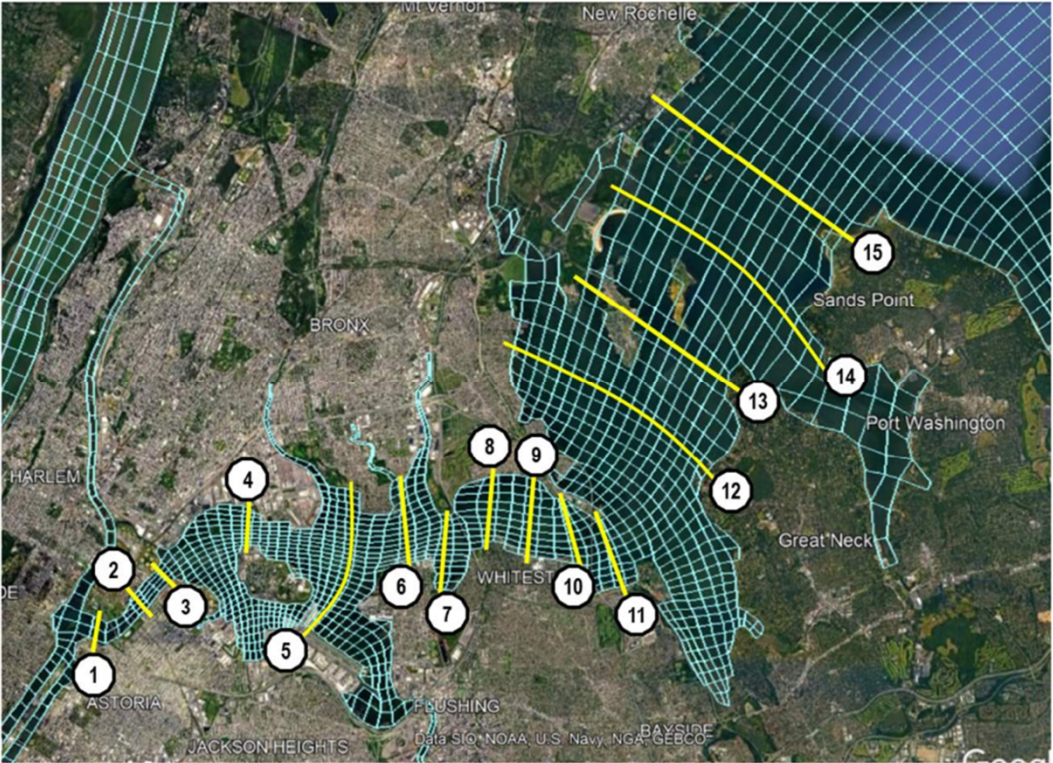
TEMPERATURE/SALINITY



CURRENT SPEEDS

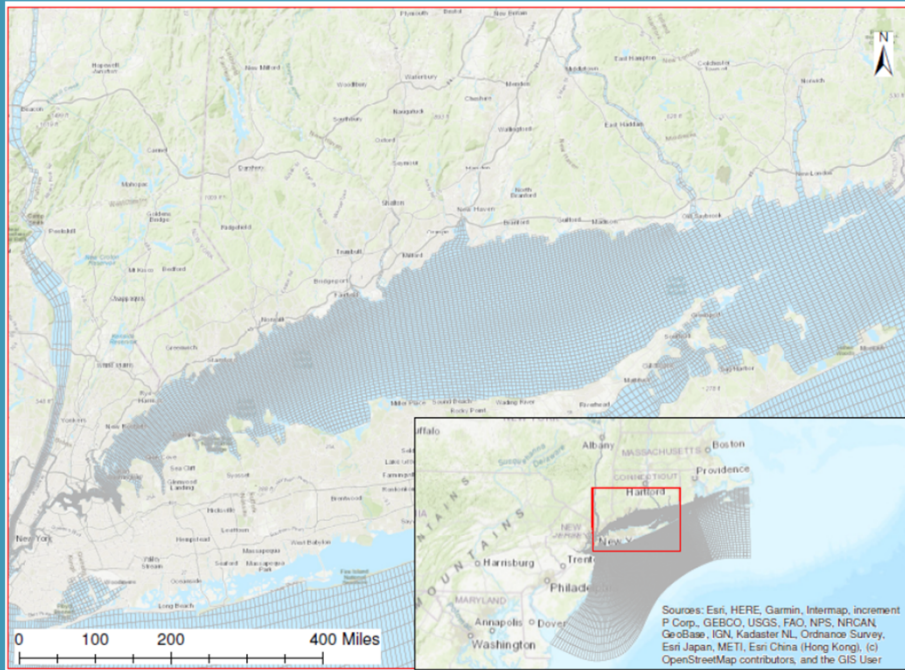


EAST RIVER FLUXES



ROMS HYDRODYNAMIC MODEL

- Model is well calibrated to available data
- Areas for improvement & data gaps
 - East River circulation & fluxes (add'l ADCP data available in 2020-21)
 - Western LIS mixing events (wind-driven) – related to onset of vertical stratification
 - Shallow water bathymetry (potentially turn on wetting/drying option to avoid minimum water depth)



01 LIS MODEL OVERVIEW

02 ROMS HYDRODYNAMIC MODEL

03 RCA WATER QUALITY MODEL

04 ROMS-RCA DETAILS

RCA MODEL HISTORY

- Initial time-variable water quality model, WASP (Water Analysis Simulation Program), developed at Hydrosience in the late 1970s
 - Generalized transport but application specific kinetic subroutine
- Provided to EPA in early 1980s (WASP8 current version)
- Hydrosience decided to maintain WASP framework but renamed it AESOP (Advanced Ecological Systems mOdeling Program) with FABLE kinetic subroutine
- In 1985, HydroQual began coupling ECOM (hydrodynamic model) and AESOP resulting in the RCA water quality model (Row Column AESOP)

MASS BALANCE FRAMEWORK

- RCA formulates mass balance equations for each model cell & state variable
- Mass balance equations include horizontal, lateral & vertical components of advective flow, dispersive mixing, & physical/chemical/biological transformations
- Includes various model inputs/loads (point & nonpoint sources)

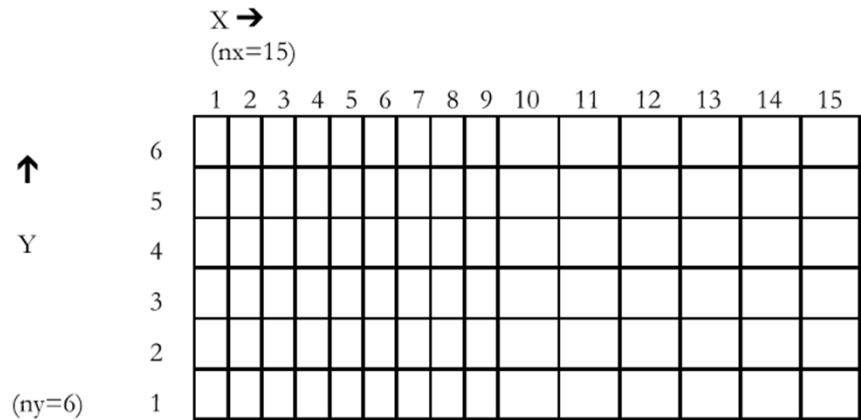
$$\frac{\partial c}{\partial t} = \underbrace{\frac{\partial}{\partial x} \left(E_x \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(E_y \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(E_z \frac{\partial c}{\partial z} \right)}_{\text{dispersive transport}} - \underbrace{U_x \frac{\partial c}{\partial x} - U_y \frac{\partial c}{\partial y} - U_z \frac{\partial c}{\partial z}}_{\text{advective transport}} + \underbrace{\pm S(x, y, z, t)}_{\text{sources or sinks}} + \underbrace{W(x, y, z, t)}_{\text{external inputs}} \quad (1-1)$$

where:

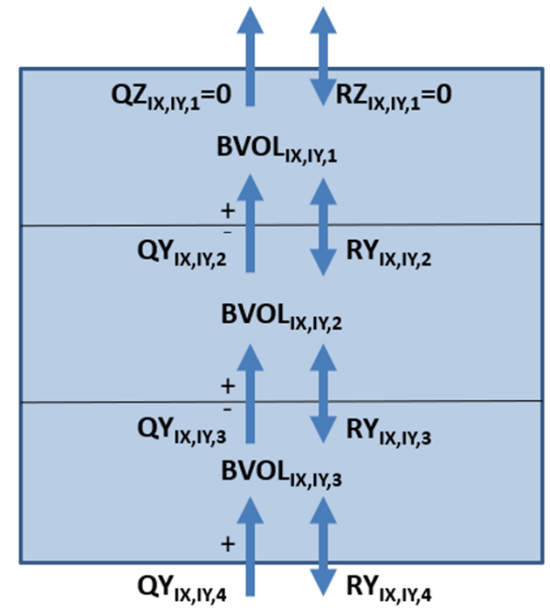
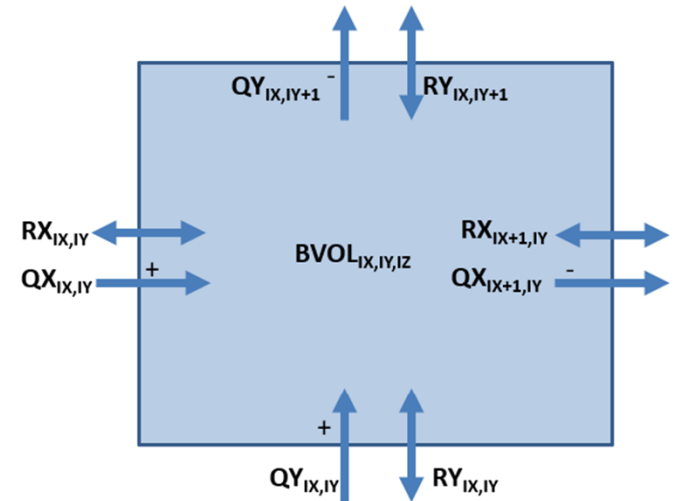
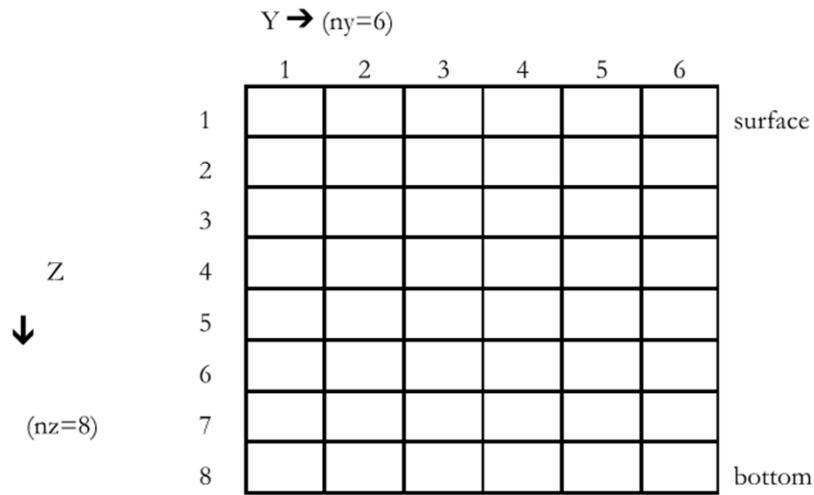
c	=	concentration of the water quality variable [M/L ³],
t	=	time [T],
E	=	dispersion (mixing) coefficient due to tides and density and velocity gradients (L ² /T),
U	=	advective velocity (L/T),
S	=	sources and sinks of the water quality variable, representing kinetic interactions (M/L ³ -T),
W	=	external inputs of the variable c (M/L ³ -T),
x,y,z	=	longitudinal, lateral and vertical coordinates,
M,L,T	=	units of mass, length and time, respectively.

MODEL SEGMENTATION

- Horizontal (X-Y) Plane

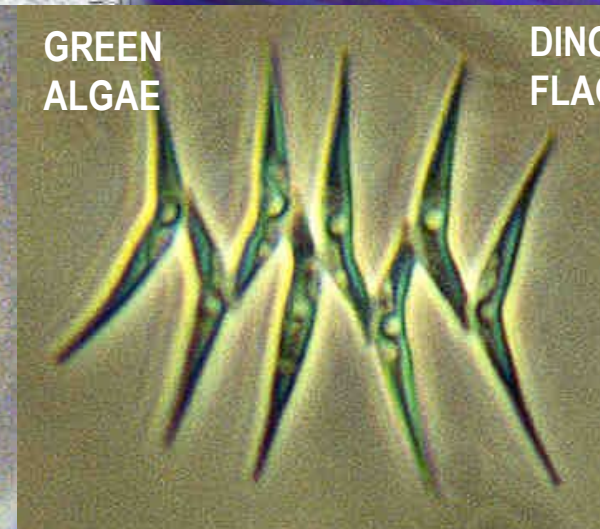
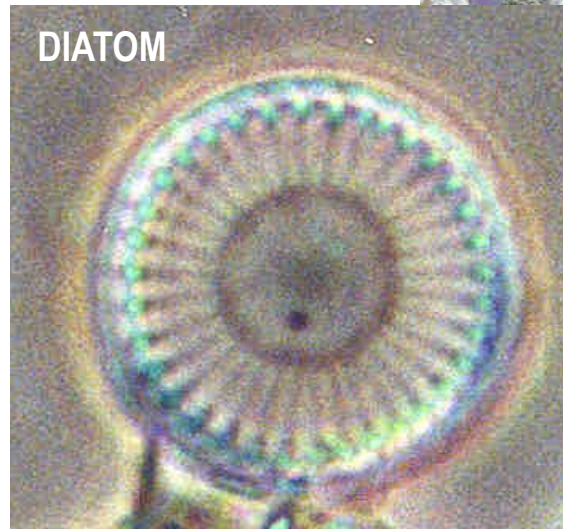
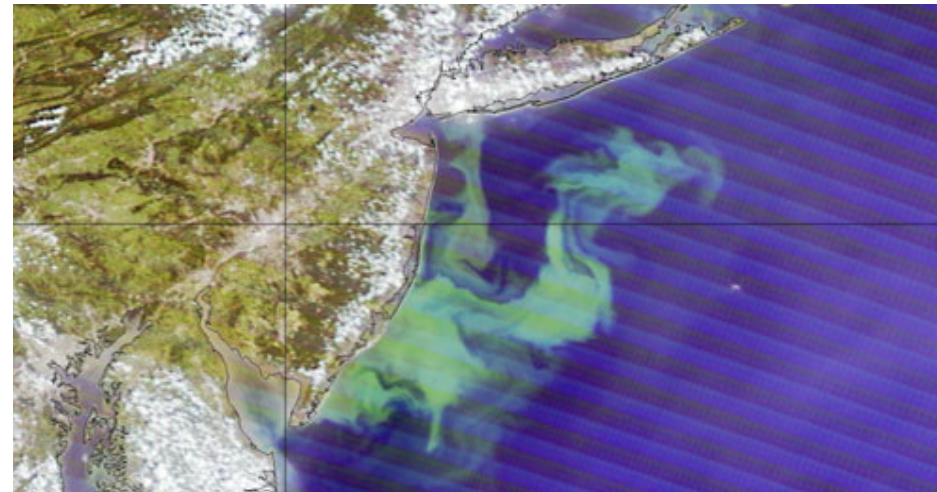


- Vertical (Z) Plane



WATER QUALITY (EUTROPHICATION) KINETICS

- Light, nutrients & grazing/predation control phytoplankton growth (and residence time)
- Phytoplankton are the base of the food-chain (i.e., ocean fisheries)
- During photosynthesis, phytoplankton convert CO_2 to organic matter (carbon cycle)
- High nutrient levels can result in over-enrichment (eutrophication)
 - Harmful algal blooms (HABs)
 - Low DO (hypoxia)
 - Aesthetic & odor problems



MODEL INPUTS

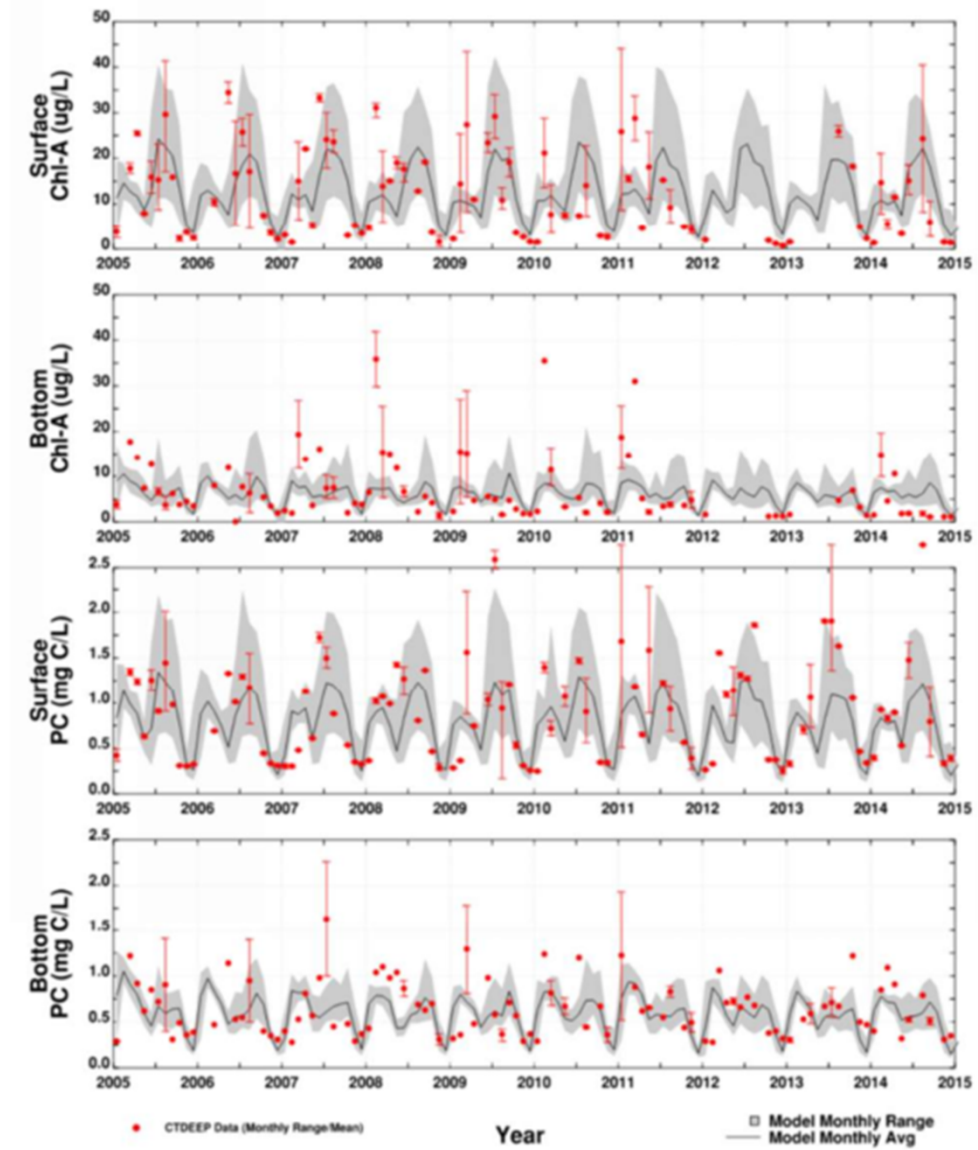
- RCA model directly coupled with ROMS
 - RCA run at same as ROMS (not separately like ECOM and RCA)
- RCA uses same model grid as ROMS
- WQ variable concentrations associated with:
 - Rivers (freshwater inputs)
 - WWTPs, CSOs, SW
 - Groundwater
- Meteorological (solar radiation – for phytoplankton growth)
- Numerous constants (phytoplankton growth/respiration rates, carbon oxidation, nitrification)

MODEL CALIBRATION/VALIDATION

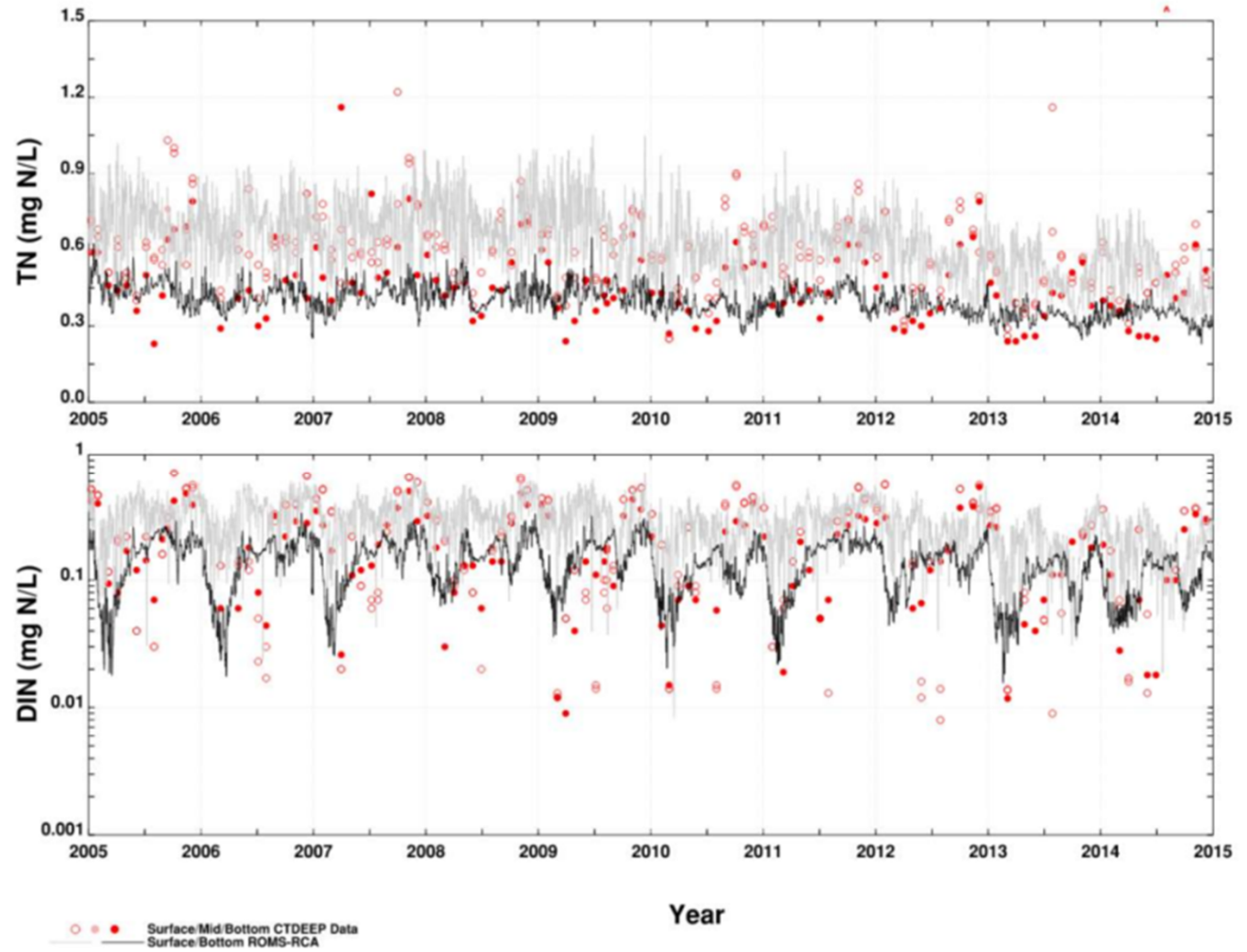
- Model output compared to data for:
 - Phytoplankton (chlorophyll-a)
 - DO
 - Nutrients (organic & inorganic)
 - TN, PON, DON, NH₄, NO₂
 - TP, POP, DOP, PO₄
 - Carbon
 - TOC, POC, DOC
 - TSS

- Datasets used:
 - CTDEEP, NYCDEP Harbor Survey, IEC, NJHDG, LISICOS
 - Research studies (phytoplankton P/R, SOD & nutrient fluxes)

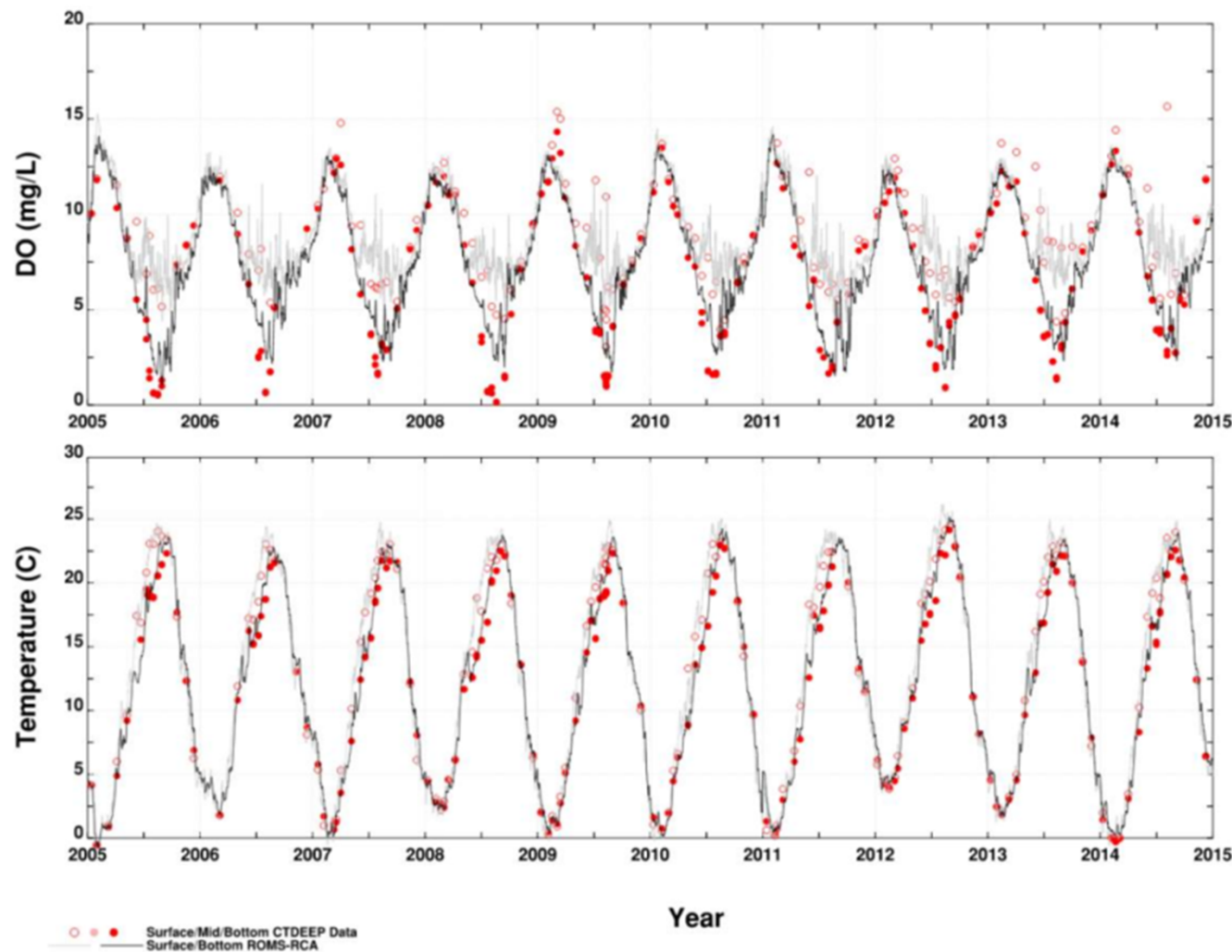
CHL-A & POC



TN & DIN

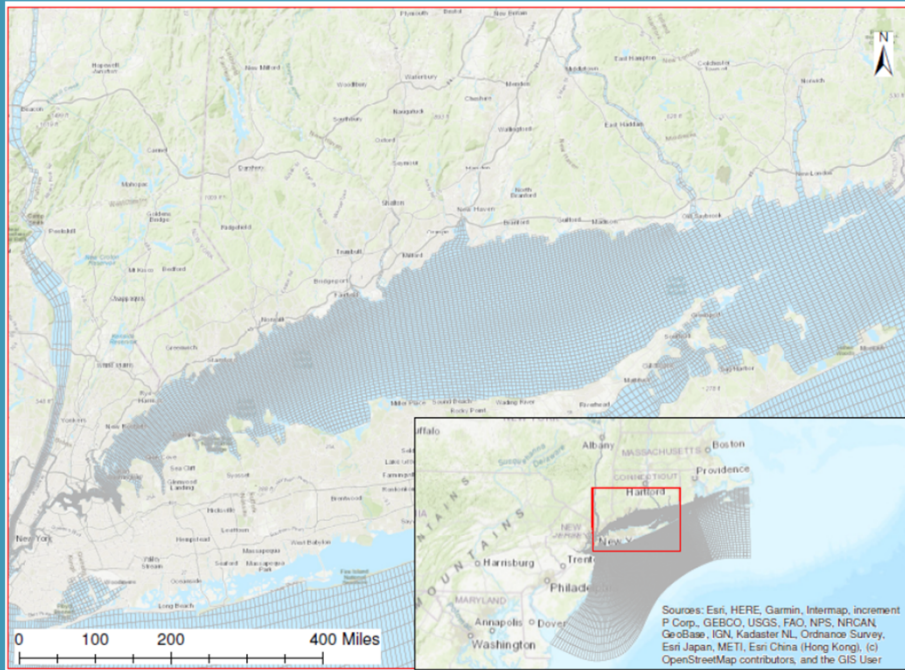


DO & TEMP



RCA WATER QUALITY MODEL

- Model is well calibrated to available data
- Areas for improvement & data gaps
 - East River circulation & fluxes (add'l ADCP data available in 2020-21) – ROMS
 - Western LIS mixing events (wind-driven) – related to onset of vertical stratification – ROMS
 - Phytoplankton production & respiration (spatial variability, East River)
 - Winter/spring algal bloom (drives low summer DO)
 - East River/western LIS focus



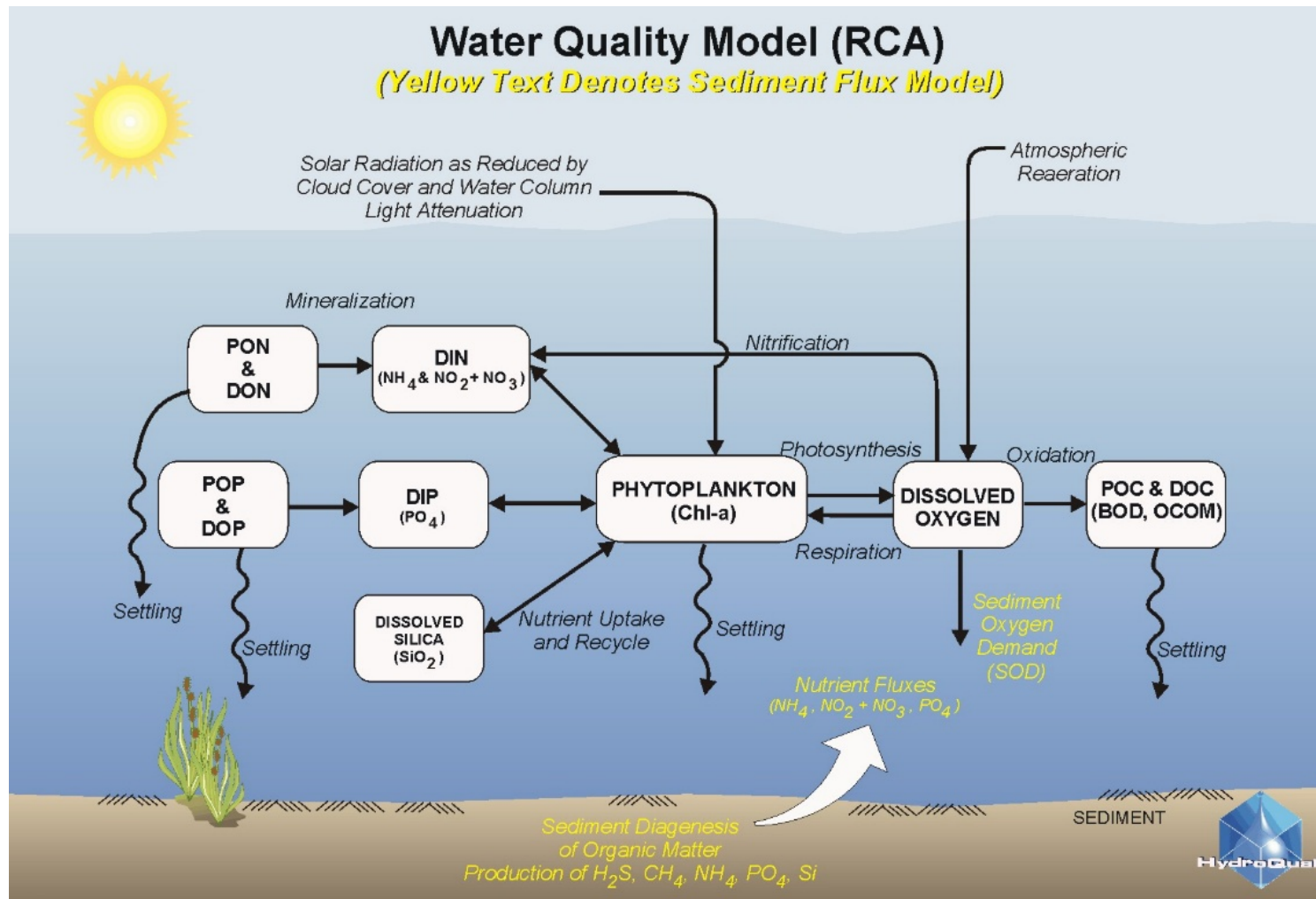
01 LIS MODEL OVERVIEW

02 ROMS HYDRODYNAMIC MODEL

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04 ROMS-RCA DETAILS

RCA WATER QUALITY MODEL KINETICS



RCA MODEL VARIABLES

State-Variable	Abbreviation	State-Variable	Abbreviation
Phytoplankton Group 1 (winter)	PHYT1	Nitrite + Nitrate Nitrogen	NO23
Phytoplankton Group 2 (summer)	PHYT2	Biogenic Silica	BSI
Phytoplankton Group 3 (spring)	PHYT3	Available Dissolved Silica	DSI
Refractory Particulate Organic Phosphorus	RPOP	Refractory Particulate Organic Carbon	RPOC
Labile Particulate Organic Phosphorus	LPOP	Labile Particulate Organic Carbon	LPOC
Refractory Dissolved Organic Phosphorus	RDOP	Reactive Particulate Organic Carbon	RePOC
Labile Dissolved Organic Phosphorus	LDOP	Refractory Dissolved Organic Carbon	RDOC
Total Phosphate	PO4T	Labile Particulate Organic Carbon	LDOC
Refractory Particulate Organic Nitrogen	RPON	Reactive Particulate Organic Carbon	ReDOC
Labile Particulate Organic Nitrogen	LPON	Algal Exudate	EXDOC
Refractory Dissolved Organic Nitrogen	RDON	Aqueous SOD	O2EQ
Labile Dissolved Organic Nitrogen	LDON	Dissolved Oxygen	DO
Total Ammonium Nitrogen	NH4T	Total Suspended Solids	TSS

PHYTOPLANKTON GROWTH & LOSS

- Source term (S_P) = [Growth rate (G_P) – Loss rate (D_P)] x Phytoplankton carbon (P_C)
 - $S_P = (G_P - D_P) \times P_C$ [=] mgC/L-day or gC/m³-day

- $G_P = G_{P_{\max}} \times G_T(T) \times G_I(I) \times G_N(N)$
 - $G_{P_{\max}}$ – maximum growth rate (1/d)
 - $G_T(T)$ – temperature effect (uses temperature optimum approach)
 - $G_I(I)$ – light limitation (function of solar radiation, fraction daylight, water depth, light attenuation)
 - $G_N(N)$ – nutrient limitation (minimum of DIN, DIP, DSi)

- $D_P = k_{PR}(T) + k_{SP} + k_{grz}$
 - $k_{PR}(T)$ – respiration (1/d)
 - k_{SP} – settling (1/d)
 - k_{grz} – grazing/predation (1/d)

GROWTH – TEMPERATURE EFFECT

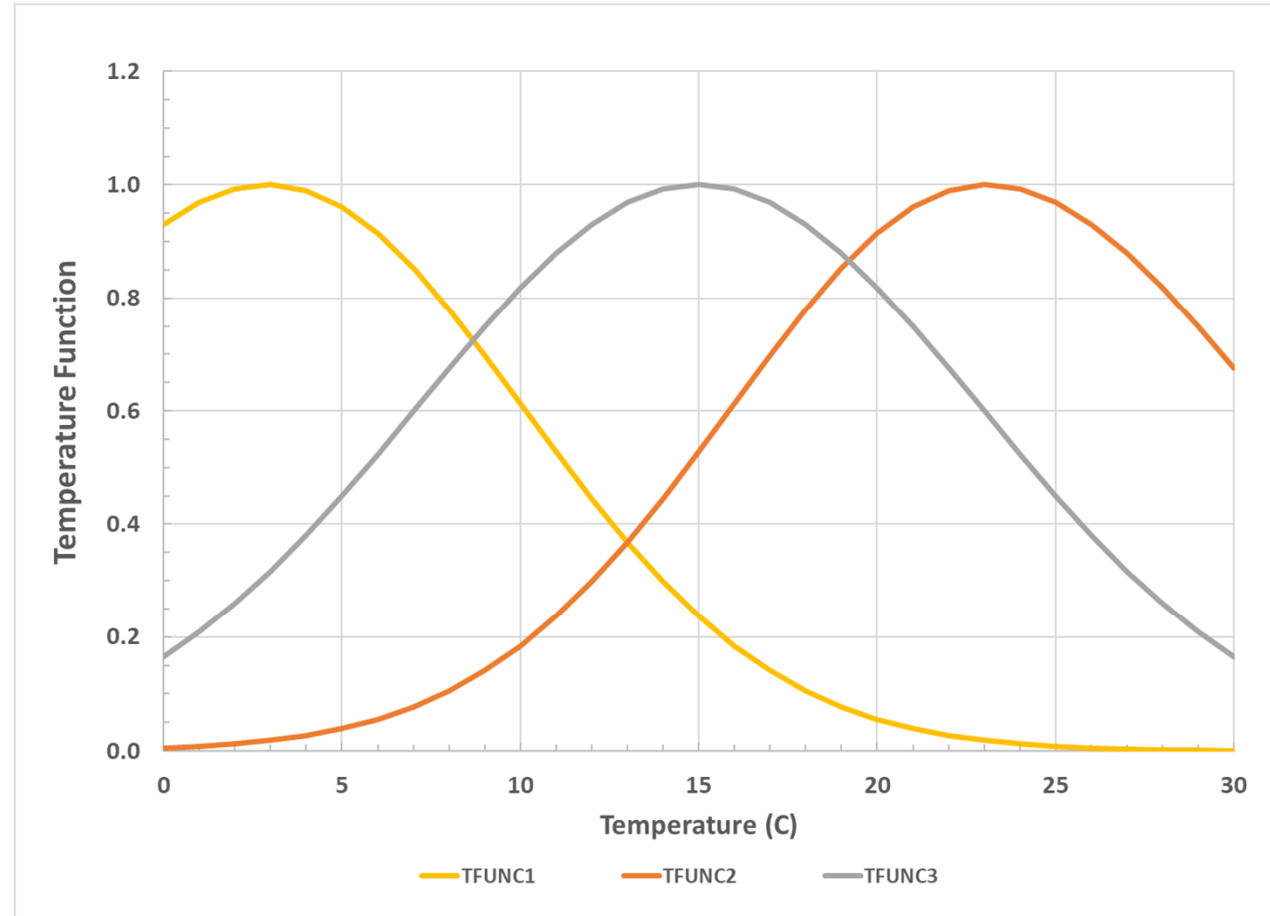
$$G_{P_{\max}}(T) = G_{P_{\max}} e^{-\beta_1 (T_{\text{opt}} - T)^2}$$

or

$$G_{P_{\max}}(T) = G_{P_{\max}} e^{-\beta_2 (T - T_{\text{opt}})^2}$$

$$T \leq T_{\text{opt}}$$

$$T > T_{\text{opt}}$$



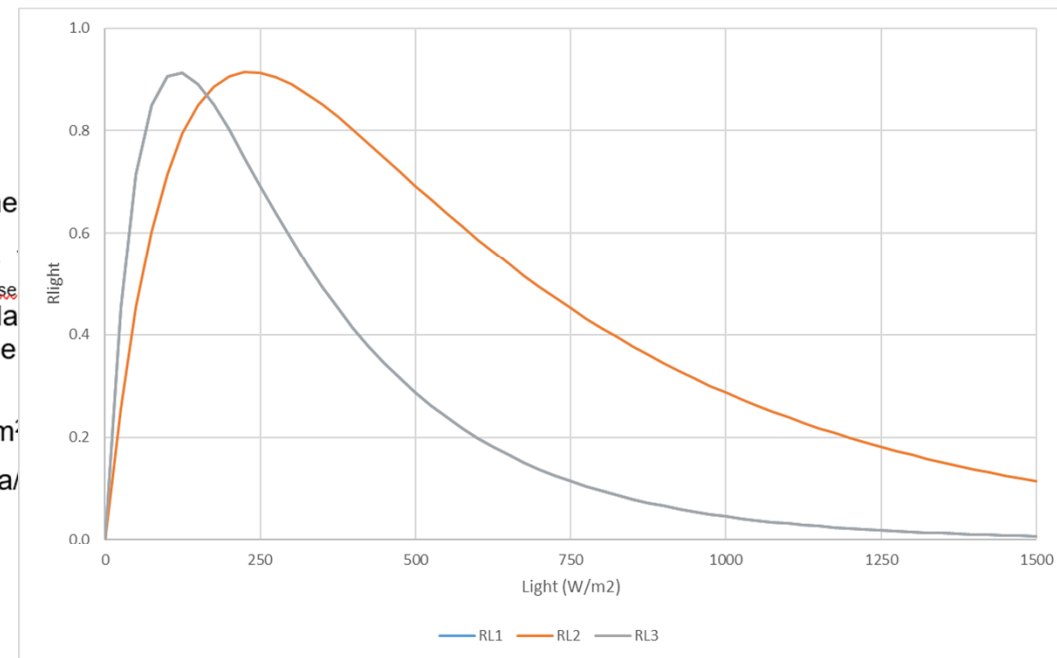
GROWTH – LIGHT LIMITATION

- Surface light limitation for attenuation of 0.5/m

$$G_I(I) = \frac{e}{k_e H} \left[\exp\left(\frac{-I_o(t)}{I_s} e^{-k_e H}\right) - \exp\left(\frac{-I_o(t)}{I_s}\right) \right]$$

where:

- e = 2.718
- H = the water column depth or thickness of the water cell or segment
- k_e = the total extinction coefficient, $k_{base} + k_c P_{chl-a} + k_{TSS} TSS$ computed from the sum of the base light attenuation, k_{base} shading attenuation due to the ambient phytoplankton population light attenuation due to total suspended solids, $k_{TSS} TSS$ and the due to CDOM, $k_{CDOM} CDOM$.
- k_c = the algal related extinction coefficient per unit of chlorophyll (m^2/mg)
- P_{chl-a} = the ambient phytoplankton population as chlorophyll ($mg\ chl-a/L$)
 $= P_c / a_{cchl}$
- P_c = the ambient phytoplankton population as carbon ($mg\ C/L$),
- a_{cchl} = the ratio of algal carbon to algal chlorophyll ($mg\ C/mg\ chl-a$),
- k_{TSS} = light attenuation due to total suspended solids ($m^2/mg\ TSS$).
- k_{CDOM} = light attenuation due to CDOM ($m^2/unit\ of\ CDOM$)
- I_o = the incident light intensity at the segment surface (ly/day),
- I_s = the saturating light intensity (ly/day).



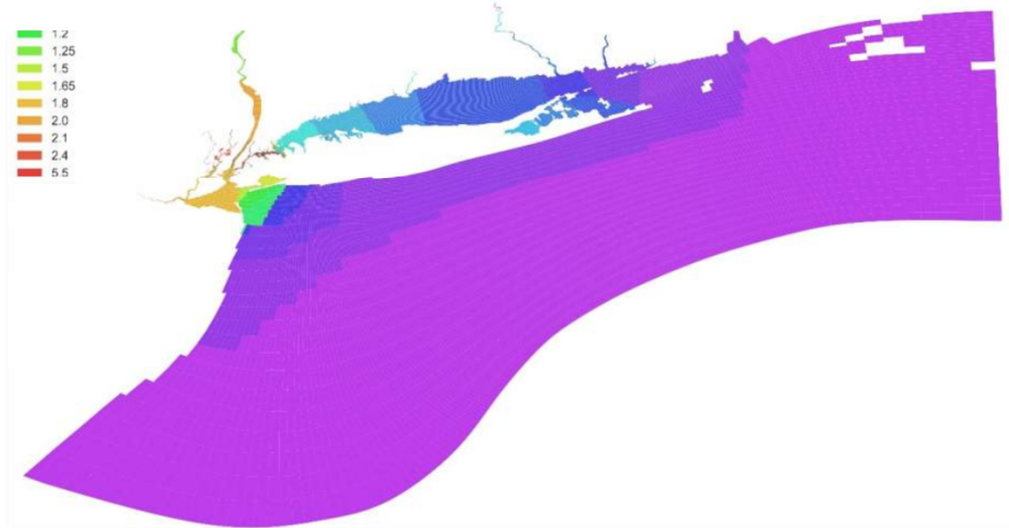
LIGHT ATTENUATION

- Light attenuation (K_e) calculated in model (function of chl-a, TSS & salinity as a proxy for CDOM)
- Equation developed using available data & a spatially variable base coefficient

$$K_e = K_{e_{base}} + 0.017 \times Chla + 0.009 \times TSS - 0.015 \times Sal$$

KEBSTVF Map

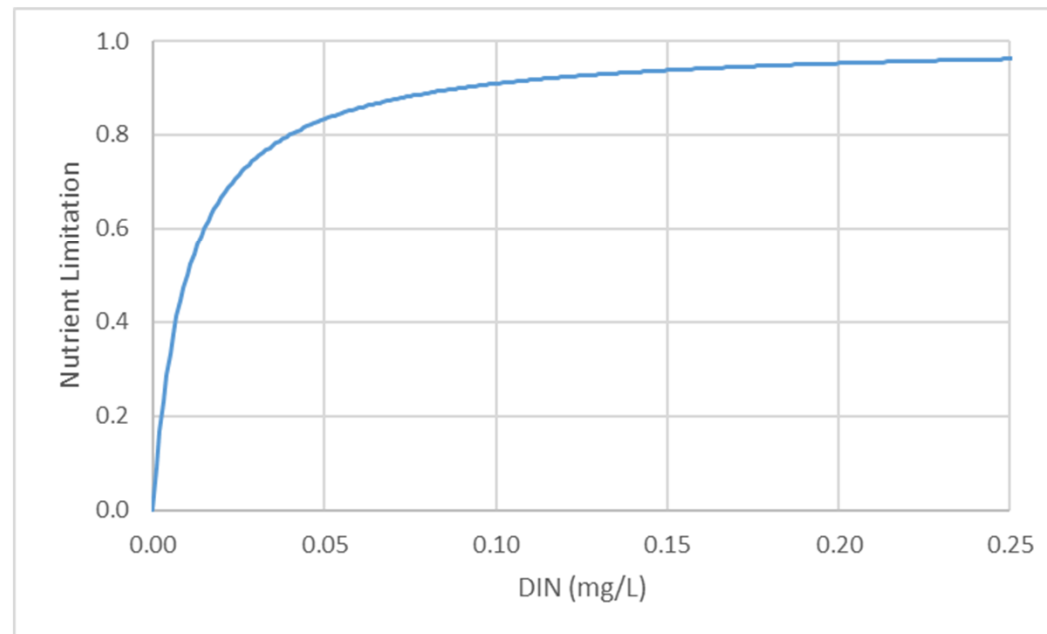
where K_e is the total light extinction coefficient and $K_{e_{base}}$ is the spatially variable base light existing coefficient. A minimum K_e of 0.3/m was also used together with this equation.



GROWTH – NUTRIENT LIMITATION

- Uses a Michaelis-Menton relationship w/ a half-saturation constant
 - Nutrient limitation is half when nutrient concentration equals half-saturation constant

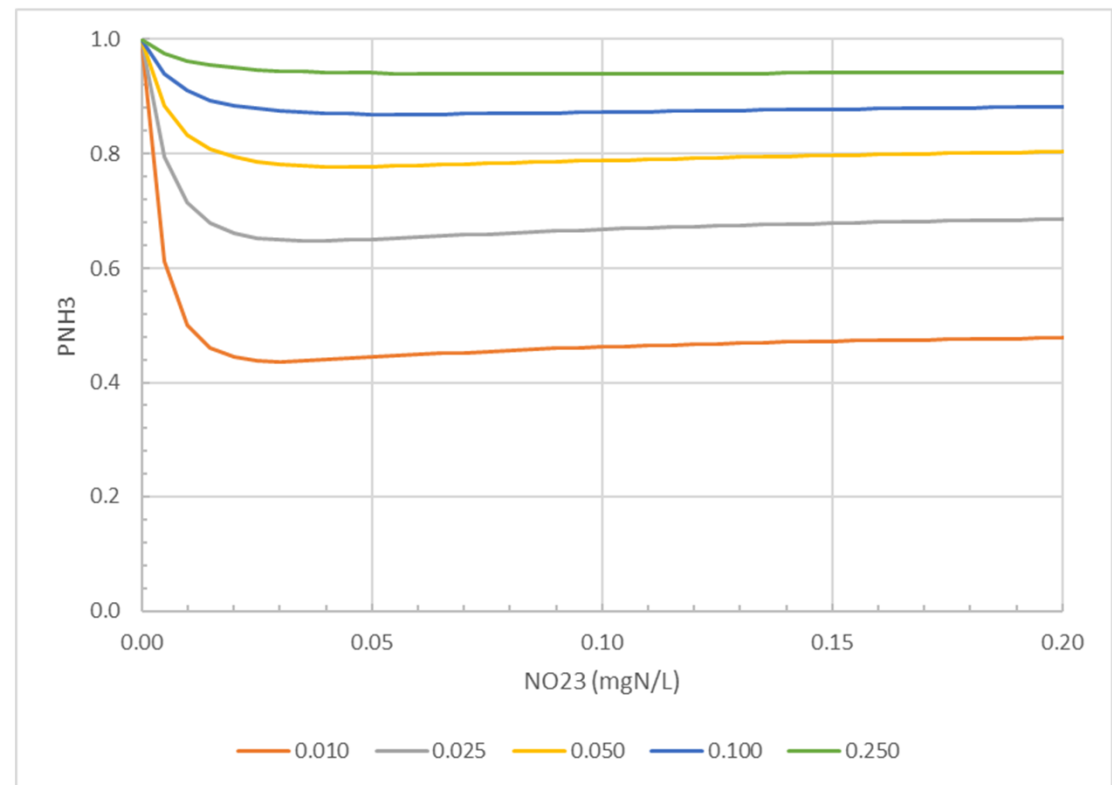
$$G_N(N) = \text{Min} \left(\frac{\text{DIN}}{K_{mN} + \text{DIN}}, \frac{\text{DIP}}{K_{mP} + \text{DIP}}, \frac{\text{Si}}{K_{mSi} + \text{Si}} \right)$$



GROWTH – AMMONIA PREFERENCE

- Phytoplankton preferably use ammonia for growth over nitrite+nitrate
 - Ammonia preference formulation is used
 - Higher preference factor when ammonia levels are high

$$\alpha_{\text{NH}_4} = \text{NH}_4 \cdot \frac{\text{NO}_3}{(\text{K}_{\text{mN}} + \text{NH}_4) \cdot (\text{K}_{\text{mN}} + \text{NO}_3)} + \text{NH}_4 \cdot \frac{\text{K}_{\text{mN}}}{(\text{NH}_4 + \text{NO}_3) \cdot (\text{K}_{\text{mN}} + \text{NO}_3)}$$



LOSS – RESPIRATION

- Uses two components (basal/resting & losses during photosynthesis)
 - r_b – basal/resting respiration rate (1/d)
 - r_g – fraction algal growth lost to energy for photosynthesis
 - G_p – phytoplankton growth rate (1/d)
 - θ_{PR} – temperature correction coefficient

$$k_{PR}(T) = r_g G_p + r_b \theta_{PR}^{T-20}$$

LOSS – SETTLING

- Uses two components (base settling & nutrient dependent settling)
 - V_{sPb} – base settling rate (m/d)
 - V_{sPn} – nutrient dependent settling (m/d)
 - $G_N(N)$ – nutrient limitation factor
 - θ_{base} – temperature correction coefficient
 - H – water depth (m)
 - k_{sP} – phytoplankton settling loss rate (1/d)

$$k_{sP} = \left[\frac{V_{sPb}}{H} + \frac{V_{sPn}}{H} \cdot (1 - G_N(N)) \right] \cdot \theta_{base}^{(T-20)}$$

LOSS – PREDATION

- LIS model implemented a new phytoplankton grazing/predation formulation
 - Provides for faster cycling of carbon due to predation
 - Significantly improved model DO calibration

$$PR = \alpha \times F \times B^2 \text{ or } \delta \times B^2$$

where: PR – phytoplankton predation (g biomass C/m³/day)

F – clearance/filtration rate (m³/g predator C/day)

B – phytoplankton biomass (g biomass C/m³)

δ – product of $\alpha \times F$ (m³/g biomass C/day)

PHYTOPLANKTON CARBON:CHL-A RATIO

- Phytoplankton levels are measured using chlorophyll-a (chl-a)
- Model calculates phytoplankton as carbon so need to convert for comparison to data
- LIS model implemented a new variable C:Chl-a ratio formulation
 - Typically, a constant C:Chl-a ratio is used (e.g., 50:1)
 - Function of light attenuation (higher C:Chl-a ratio when water is clearer)

$$C/Chla = a + b \times \exp(-c \times K_e)$$

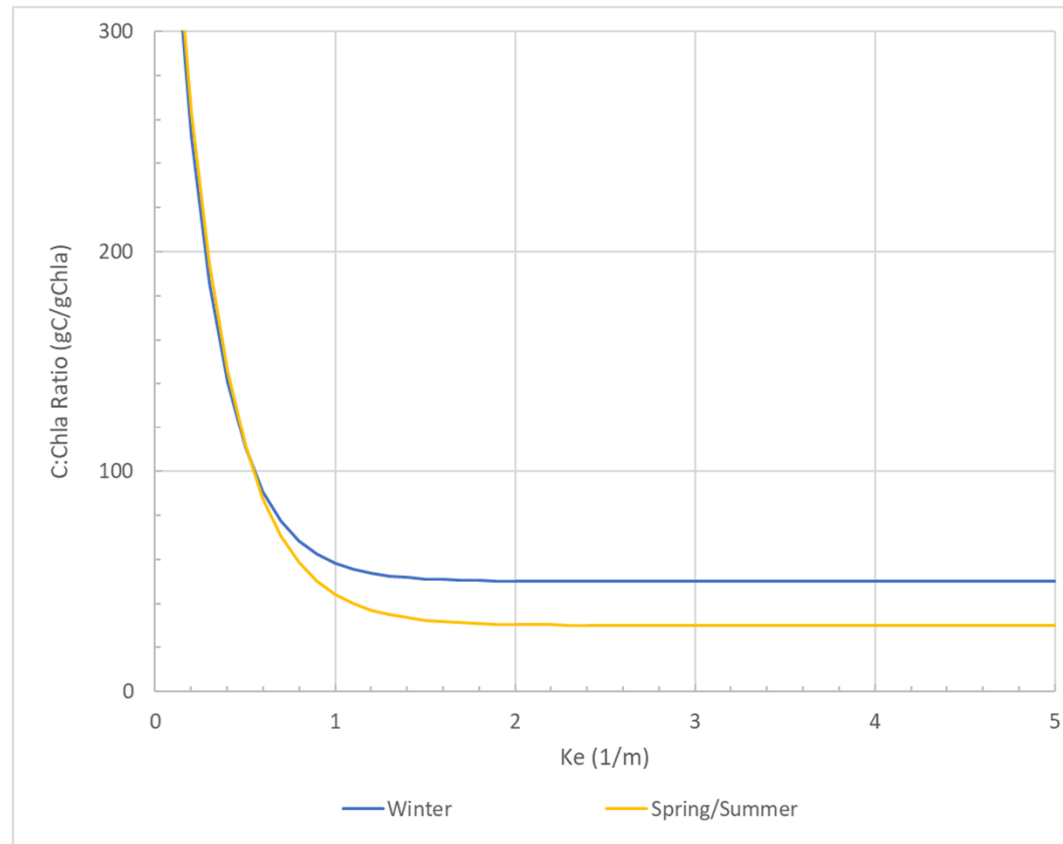
where: a = 50 (winter algal group), 30 (summer and spring algal groups)

b = 450 (winter algal group), 470 (summer and spring algal groups)

c = 4.0 (winter algal group), 3.5 (summer and spring algal groups)

PHYTOPLANKTON CARBON:CHL-A RATIO

- LIS light attenuation ranges from 0.5-0.75/m



PHYTOPLANKTON NUTRIENT STOICHIOMETRY

- Uses a variable stoichiometry approach as a function of ambient nutrient levels
 - Phytoplankton use less nutrients for growth at low nutrient levels

$$\frac{C}{X} = X_1 + (X_2 - X_1)e^{-X_3 \cdot DIX}$$

where:

$\frac{C}{X}$ = carbon to nutrient ratio,

X_1 = nutrient saturated, carbon to nutrient ratio

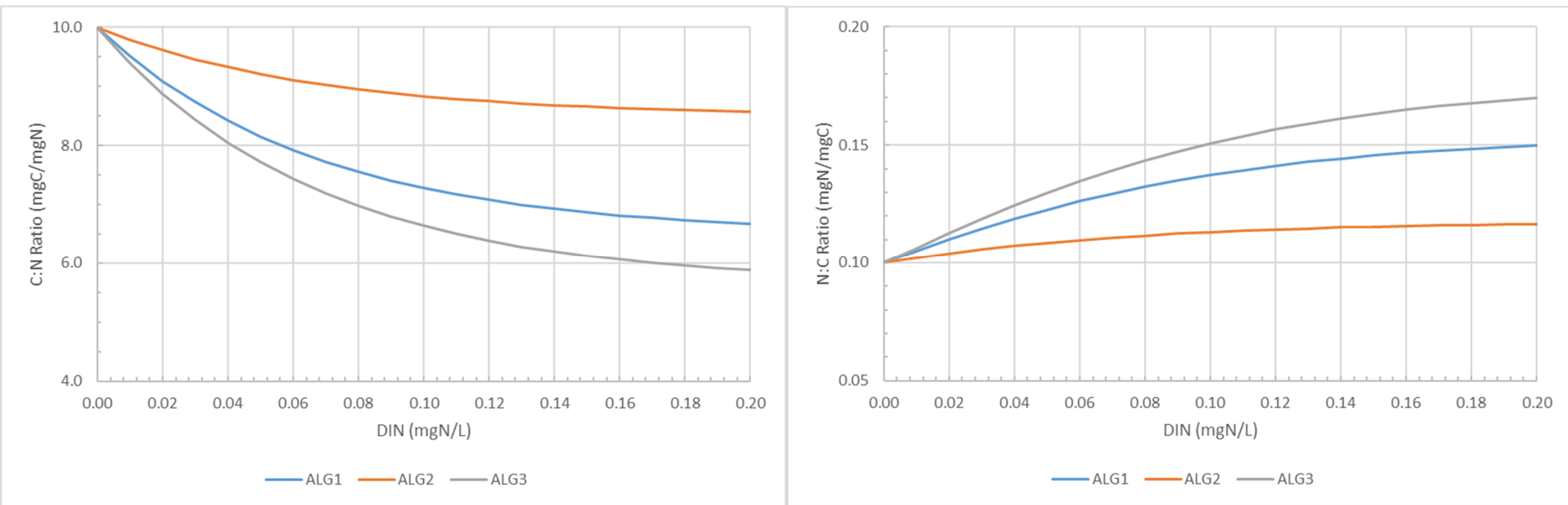
X_2 = nutrient limited, carbon to nutrient ratio (maximum),

X_3 = coefficient that determines the rate at which the carbon to nutrient ratio changes as a function of the ambient nutrient concentration, DIX,

DIX = dissolved concentration of available nutrient (either DIN, DIP, or DSi)

PHYTOPLANKTON NUTRIENT STOICHIOMETRY

- Less nutrient uptake per unit phytoplankton carbon at low nutrient levels

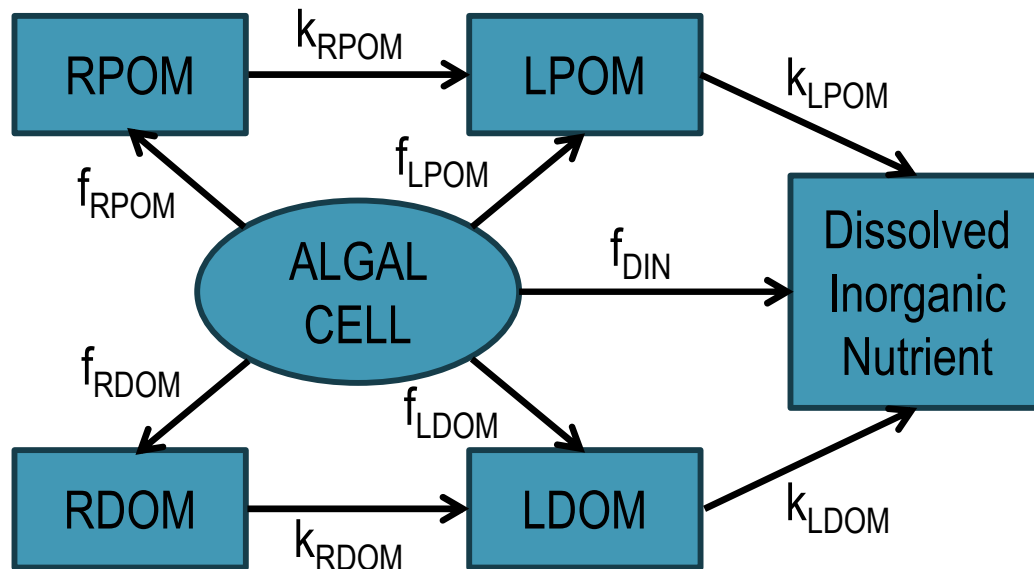


ORGANIC MATTER (N/P/C)

- Model uses particulate & dissolved fractions along with different reactivities
 - Refractory particulate
 - Labile particulate
 - Refractory dissolved
 - Labile dissolved
- Refractory – hydrolysis & mineralization rate $\sim 0.005\text{-}0.01/\text{d}$ (half-life $\sim 70\text{-}140$ days)
- Labile – hydrolysis & mineralization rate $\sim 0.05\text{-}0.10/\text{d}$ (half-life $\sim 7\text{-}14$ days)
- Two additional reactivity classes for organic carbon
 - Reactive POC & DOC (used mainly for CSO sources)
 - Rate used = $0.15/\text{d}$ (half-life = 5 days)

CARBON & NUTRIENT CYCLING

- Nutrients are utilized by phytoplankton for growth (nutrient uptake)
- Due to grazing/predation (fecal pellets or unassimilated particulate matter) & respiration, nutrients are returned (in various forms) to the water column
- Carbon cycled due to grazing/predation



Fraction	Carbon	Nitrogen	Phosphorus
f_{RPOM}	0.05	0.05	0.05
f_{LPOM}	0.25	0.10	0.10
f_{RDOM}	0.05	0.05	0.05
f_{LDOM}	0.65	0.20	0.20
f_{DIN}	-	0.60 (NH ₄)	0.60 (PO ₄)

NITROGEN

Refractory Particulate Organic Nitrogen (RPON)

$$S_{10} = a_{NC} \cdot f_{RPON} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c - k_{10,12} \theta_{10,12}^{T-20} \cdot RPON \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{V_{s10}}{H} \cdot RPON$$

Labile Particulate Organic Nitrogen (LPON)

$$S_{11} = a_{NC} \cdot f_{LPON} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c - k_{11,13} \theta_{11,13}^{T-20} \cdot LPON \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{V_{s11}}{H} \cdot LPON$$

Refractory Dissolved Organic Nitrogen (RDON)

$$S_{12} = a_{NC} \cdot f_{RDON} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c + k_{10,12} \theta_{10,12}^{T-20} \cdot RPON \cdot \frac{P_c}{K_{mP_c} + P_c} - k_{12,14} \theta_{12,14}^{T-20} \cdot RDON \cdot \frac{P_c}{K_{mP_c} + P_c}$$

Labile Dissolved Organic Nitrogen (LDON)

$$S_{13} = a_{NC} \cdot f_{LDON} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c + k_{11,13} \theta_{11,13}^{T-20} \cdot LPON \cdot \frac{P_c}{K_{mP_c} + P_c} + k_{13,14} \theta_{13,14}^{T-20} \cdot LDON \cdot \frac{P_c}{K_{mP_c} + P_c}$$

Ammonia Nitrogen (NH₄)

$$S_{14} = a_{NC} \cdot f_{NH_4} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c + (k_{12,14} \theta_{12,14}^{T-20} \cdot RDON + k_{13,14} \theta_{13,14}^{T-20} \cdot LDON) \cdot \frac{P_c}{K_{mP_c} + P_c} - a_{NC} \cdot \alpha_{NH_4} \cdot (1 - f_{ExPP}) \cdot G_P \cdot P_c - k_{14,15} \theta_{14,15}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO}$$

Nitrite + Nitrate Nitrogen (NO₂ + NO₃)

$$S_{15} = k_{14,15} \theta_{14,15}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} - a_{NC} \cdot (1 - \alpha_{NH_4}) \cdot (1 - f_{ExPP}) \cdot G_P \cdot P_c - k_{15,0} \theta_{15,0}^{T-20} \cdot NO_2 + NO_3 \cdot \frac{K_{NO_3}}{K_{NO_3} + DO}$$

PHOSPHORUS

Refractory Particulate Organic Phosphorus (RPOP)

$$S_5 = a_{PC} \cdot f_{RPOP} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c - k_{5,7} \theta_{5,7}^{T-20} \cdot RPOP \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{V_{s5}}{H} \cdot RPOP$$

Labile Particulate Organic Phosphorus (LPOP)

$$S_6 = a_{PC} \cdot f_{LPOP} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c - k_{6,8} \theta_{6,8}^{T-20} \cdot LPOP \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{V_{s6}}{H} \cdot LPOP$$

Refractory Dissolved Organic Phosphorus (RDOP)

$$S_7 = a_{PC} \cdot f_{RDOP} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c + k_{5,7} \theta_{5,7}^{T-20} \cdot RPOP \cdot \frac{P_c}{K_{mP_c} + P_c} - k_{7,9} \theta_{7,9}^{T-20} \cdot RDOP \cdot \frac{P_c}{K_{mP_c} + P_c}$$

Labile Dissolved Organic Phosphorus (LDOP)

$$S_8 = a_{PC} \cdot f_{LDOP} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c + k_{6,8} \theta_{6,8}^{T-20} \cdot LPOP \cdot \frac{P_c}{K_{mP_c} + P_c} - k_{8,9} \theta_{8,9}^{T-20} \cdot LPOP \cdot \frac{P_c}{K_{mP_c} + P_c}$$

Dissolved Inorganic Phosphorus (DIP)

$$S_9 = a_{PC} \cdot f_{DIP} \cdot (k_{PR}(T) + k_{grz}(T)) \cdot P_c + (k_{7,9} \theta_{7,9}^{T-20} \cdot RDOP + k_{8,9} \theta_{8,9}^{T-20} \cdot LDOP) \cdot \frac{P_c}{K_{mP_c} + P_c} - a_{PC} \cdot (1 - f_{ExPP}) \cdot G_P \cdot P_c$$

SILICA

Biogenic Silica (BSi)

$$S_{16} = (k_{PR}(T) + k_{grz}(T)) \cdot P_c - k_{16,17} \theta_{16,17}^{T-20} \cdot BSi \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{v_{s16}}{H} \cdot BSi$$

Available Silica (Si)

$$S_{17} = k_{16,17} \theta_{16,17}^{T-20} \cdot BSi \cdot \frac{P_c}{K_{mP_c} + P_c} - (1 - f_{EXP}) \cdot a_{sc} \cdot G_p \cdot P_c$$

CARBON

Refractory Particulate Organic Carbon (RPOC)

$$S_{18} = f_{\text{RPOC}} \cdot k_{\text{grz}}(T) \cdot P_c - k_{18,20} \theta_{18,20}^{T-20} \cdot \text{RPOC} \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{v_{s18}}{H} \cdot \text{RPOC}$$

Labile Particulate Organic Carbon (LPOC)

$$S_{19} = f_{\text{LPOC}} \cdot k_{\text{grz}}(T) \cdot P_c - k_{19,21} \theta_{19,21}^{T-20} \cdot \text{LPOC} \cdot \frac{P_c}{K_{mP_c} + P_c} - \frac{v_{s19}}{H} \cdot \text{LPOC}$$

Refractory Dissolve Organic Carbon (RDOC)

$$S_{20} = f_{\text{RDOC}} \cdot k_{\text{grz}}(T) \cdot P_c - k_{18,20} \theta_{18,20}^{T-20} \cdot \text{RPOC} \cdot \frac{P_c}{K_{mP_c} + P_c} \\ - k_{20,0} \theta_{20,0}^{T-20} \cdot \text{RDOC} \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{\text{DO}}{K_{\text{DO}} + \text{DO}}$$

Labile Dissolved Organic Carbon (LDOC)

$$S_{21} = f_{\text{LDOC}} \cdot k_{\text{grz}}(T) \cdot P_c - k_{19,21} \theta_{19,21}^{T-20} \cdot \text{LPOC} \cdot \frac{P_c}{K_{mP_c} + P_c} \\ - k_{21,0} \theta_{21,0}^{T-20} \cdot \text{LDOC} \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{\text{DO}}{K_{\text{DO}} + \text{DO}} \cdot \frac{\text{LDOC}}{K_{\text{mLDOC}} + \text{LDOC}} \\ - \frac{5}{4} \cdot \frac{12}{14} \cdot k_{15,0} \theta_{15,0}^{T-20} \cdot \text{NO}_2 + \text{NO}_3 \cdot \frac{K_{\text{NO}_3}}{K_{\text{NO}_3} + \text{DO}}$$

CARBON

Algal Exudate Dissolved Organic Carbon (ExDOC)

$$S_{22} = f_{\text{ExPP}} \cdot G_P \cdot P_c - k_{22,0} \theta_{22,0}^{T-20} \cdot \text{ExDOC} \cdot \frac{P_c}{K_{\text{mp}_c} + P_c} \cdot \frac{\text{DO}}{K_{\text{DO}} + \text{DO}} \cdot \frac{\text{ExDOC}}{K_{\text{mLDOC}} + \text{ExDOC}}$$

Reactive Particulate Organic Carbon (RePOC)

$$S_{23} = -k_{23,24} \theta_{23,24}^{T-20} \cdot \text{RePOC} \cdot \frac{P_c}{K_{\text{mp}_c} + P_c} - \min \left[v_{24 \max}, v_{24 \min} + (v_{24 \max} - v_{24 \min}) \left(\frac{\text{RePOC}}{C_{\text{ref}}} \right)^\beta \right] \cdot \text{RePOC}$$

Reactive Dissolved Organic Carbon (ReDOC)

$$S_{24} = -k_{23,24} \theta_{23,24}^{T-20} \cdot \text{RePOC} \cdot \frac{P_c}{K_{\text{mp}_c} + P_c} \cdot k_{24,0} \theta_{24,0}^{T-20} \cdot \text{ReDOC} \cdot \frac{P_c}{K_{\text{mp}_c} + P_c} \cdot \frac{\text{DO}}{K_{\text{DO}} + \text{DO}} \cdot \frac{\text{ReDOC}}{K_{\text{mLDOC}} + \text{ReDOC}}$$

DISSOLVED OXYGEN

- Phytoplankton

- By-product of photosynthetic carbon fixation is oxygen production
- Different levels of oxygen production based on use of ammonia or nitrite+nitrate
- Respiration (reverse of photosynthesis)

$$S_{25} = a_{OC} \cdot \overset{NH_3}{\alpha_{NH_4}} \cdot G_P \cdot P_c + \left(a_{NO_3} \overset{NO_2}{c} \right) \cdot (1 - \alpha_{NH_4}) \cdot G_P \cdot P_c$$

$$k_{PR}(T) = r_g G_P + r_b \theta_{PR}^{T-20}$$

- BOD (RDOC, LDOC, REDOC) oxidation

- Use of O2/C ratio = 2.67

$$-a_{OC} \cdot \left[k_{20,0} \theta_{20,0}^{T-20} \cdot RDOC + k_{21,0} \theta_{21,0}^{T-20} \cdot LDOC \cdot \frac{LDOC}{K_{mLDOC} + LDOC} \right.$$

$$+ k_{22,0} \theta_{22,0}^{T-20} \cdot ReDOC \cdot \frac{ReDOC}{K_{mLDOC} + ReDOC}$$

$$\left. + k_{23,0} \theta_{23,0}^{T-20} \cdot ExDOC \cdot \frac{ExDOC}{K_{mLDOC} + ExDOC} \right] \cdot \frac{P_c}{K_{mPc} + P_c} \cdot \frac{DO}{K_{DO} + DO}$$

- Ammonia nitrification

- Use of O2/N ratio = 4.57

$$-2 \cdot a_{ON} \cdot k_{14,15} \theta_{14,15}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO}$$

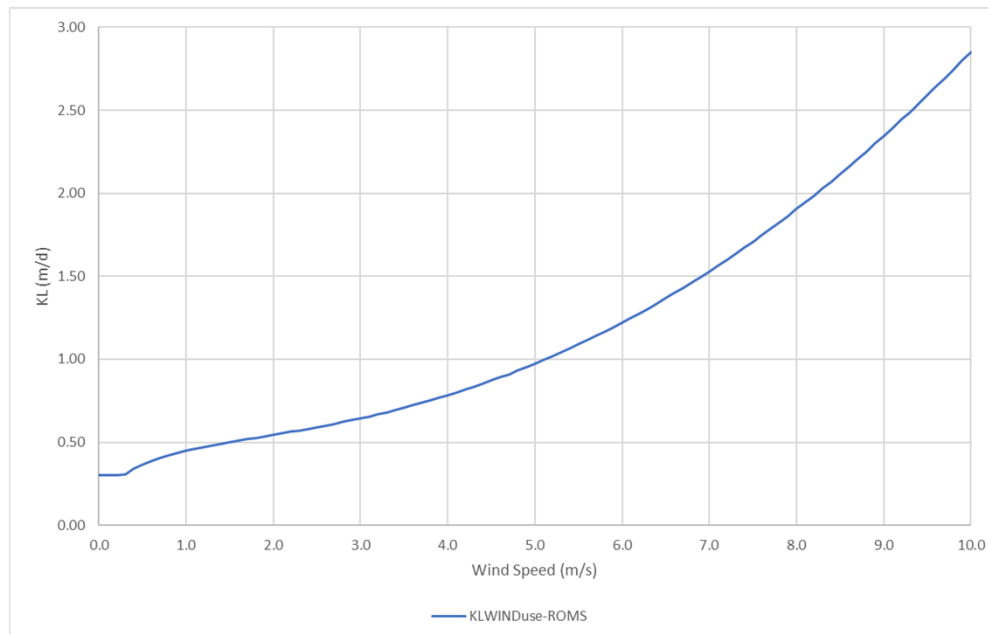
DISSOLVED OXYGEN

- Atmospheric reaeration

- Uses a wind function to calculate the oxygen transfer coefficient (K_L)

$$K_L = 0.728 \times WIND^{0.5} - 0.317 \times WIND + 0.0372 \times WIND^2$$

where $WIND$ is wind speed in m/s and K_L is the oxygen transfer coefficient (m/d).



DISSOLVED OXYGEN

Sulfide Oxygen Equivalents (O_2^*)

$$S_{24} = K_{O_2^*} \theta_{O_2^*}^{T-20} \cdot O_2^* \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO_{O_2^*}} + DO}$$

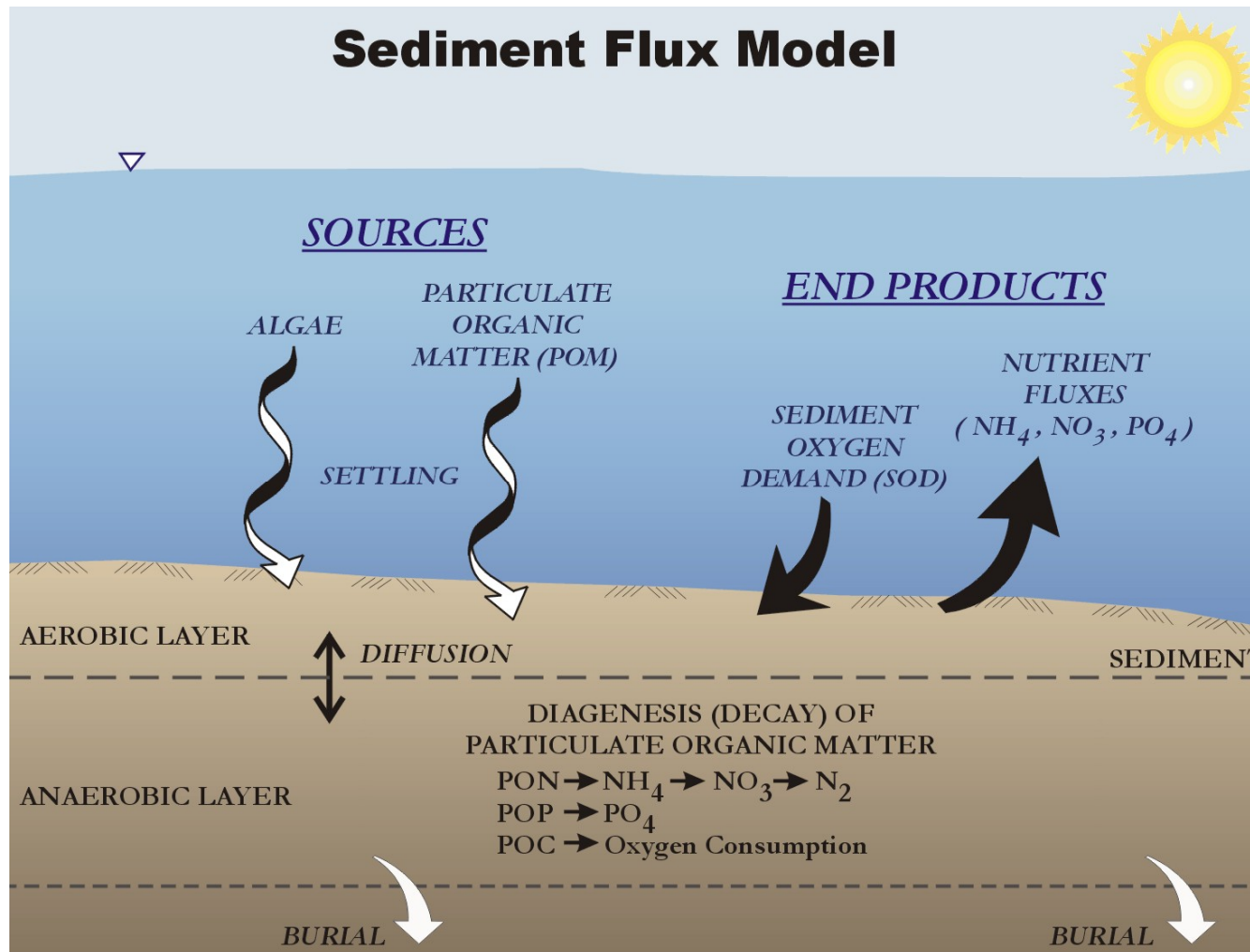
Dissolved Oxygen (DO)

NH3

NO23

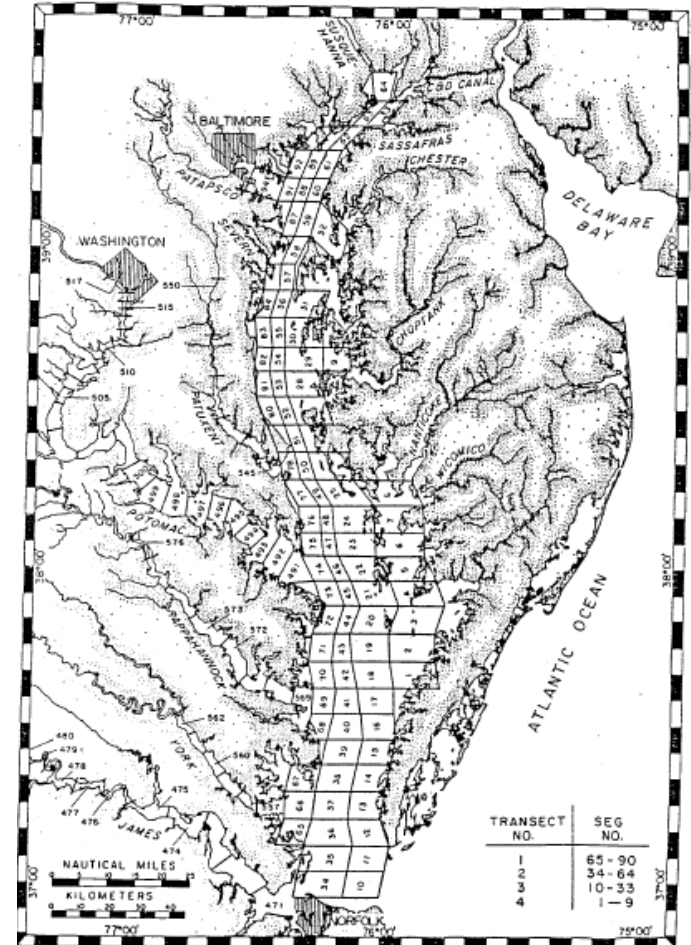
$$\begin{aligned} S_{25} = & a_{OC} \cdot \alpha_{NH_4} \cdot G_P \cdot P_c + (a_{NO_3} c) \cdot (1 - \alpha_{NH_4}) \cdot G_P \cdot P_c \\ & + k_a \theta_a^{T-20} \cdot (DO_{sat} - DO) - a_{OC} \cdot k_{PR}(T) \cdot P_c \\ & - 2 \cdot a_{ON} \cdot k_{14,15} \theta_{14,15}^{T-20} \cdot NH_4 \cdot \frac{DO}{K_{nitr} + DO} \\ & - a_{OC} \cdot \left[k_{20,0} \theta_{20,0}^{T-20} \cdot RDOC + k_{21,0} \theta_{21,0}^{T-20} \cdot LDOC \cdot \frac{LDOC}{K_{mLDOC} + LDOC} \right. \\ & + k_{22,0} \theta_{22,0}^{T-20} \cdot ReDOC \cdot \frac{ReDOC}{K_{mLDOC} + ReDOC} \\ & \left. + k_{23,0} \theta_{23,0}^{T-20} \cdot ExDOC \cdot \frac{ExDOC}{K_{mLDOC} + ExDOC} \right] \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO} + DO} \\ & - k_{O_2^*} \theta_{O_2^*}^{T-20} \cdot O_2^* \cdot \frac{P_c}{K_{mP_c} + P_c} \cdot \frac{DO}{K_{DO_{O_2^*}} + DO} \end{aligned}$$

RCA SEDIMENT FLUX SUBMODEL



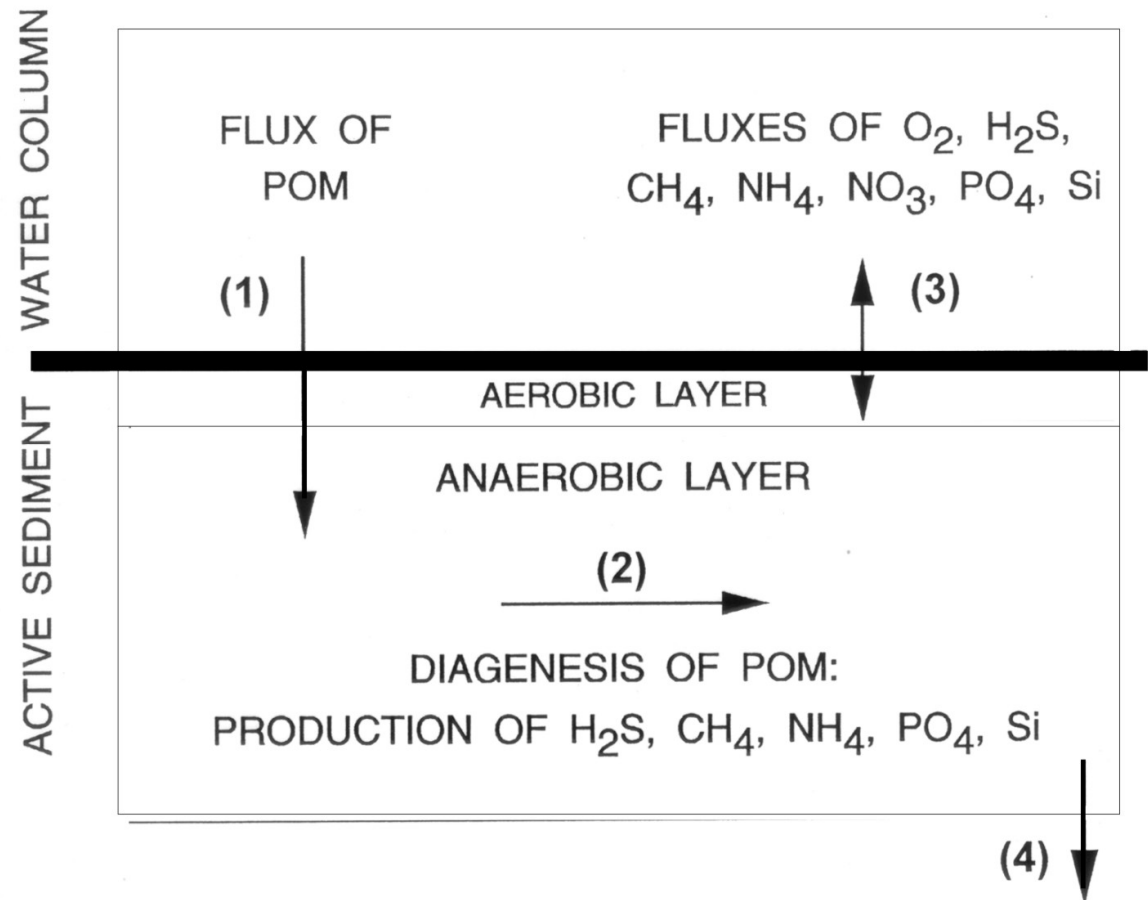
WHY USE A SEDIMENT FLUX MODEL (SFM)

- Historically, sediment bed was treated as a boundary condition, with sediment oxygen demand (SOD) and nutrient fluxes specified based on observed data
- Early modeling on Chesapeake Bay changed all that
 - Point source (PS) reduction scenario did not affect bay WQ
 - PS reductions decreased phytoplankton biomass, which in turn decreases SOD and nutrient fluxes
 - This process was not recognized with fixed SOD/nutrient fluxes
- Sediment flux model was developed to address this issue



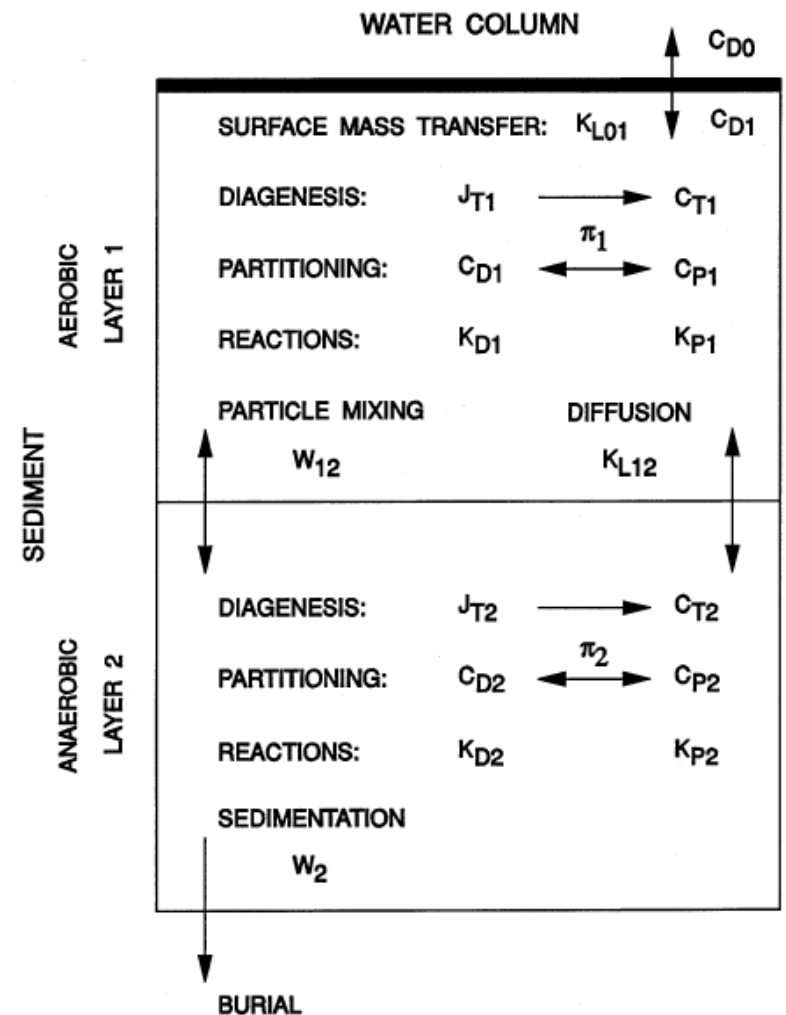
SFM FRAMEWORK

- SFM accounts for
 - Deposition of POM (1)
 - Diagenesis/decomposition of POM (2)
 - Flux of SOD and inorganic nutrient end-products based to water column (3)
 - Burial to deep sediments (4)
- Includes aerobic & anaerobic layers



SFM FRAMEWORK

- Diagenesis assumed to occur at same rate in aerobic & anaerobic sediment layers
- PO₄ & Si can sorb to solids in both layers but stronger partitioning in aerobic layer due to iron oxides
 - Weak NH₄ partitioning
- Nitrification only occurs in the aerobic layer
- Denitrification occurs in the anaerobic layer producing N₂ gas (small amount occurs in aerobic layer anoxic zones)
- No reactions for PO₄ and Si (only loss is through flux to water column & burial)



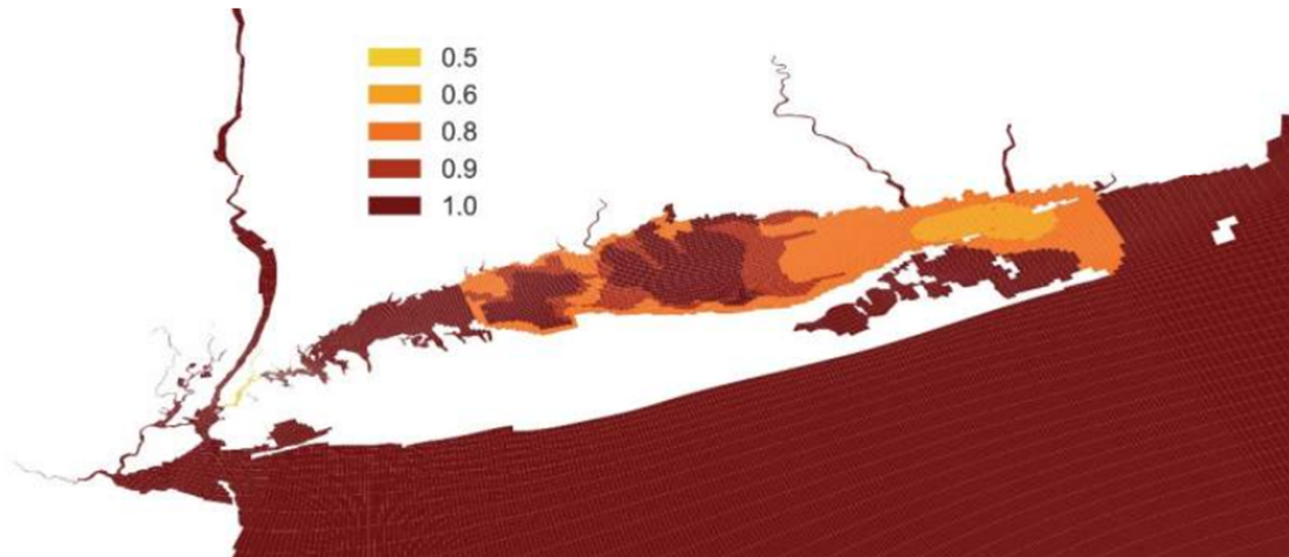
SEDIMENT REACTIVITY CLASSES

- Uses multi-class G model (3 classes used – G1, G2, G3)
 - G1 diagenesis rate = 0.035/d (half-life ~20 days)
 - G2 diagenesis rate = 0.0018/d (half-life ~1 year)
 - G3 diagenesis rate = 1.0e-06/d (basically inert)

- Settling POM & phytoplankton split into the different G classes
 - G1 – labile POM (100%) + 65% phytoplankton
 - G2 – refractory POM (57%) + 20% phytoplankton
 - G3 – refractory POM (43%) + 15% phytoplankton

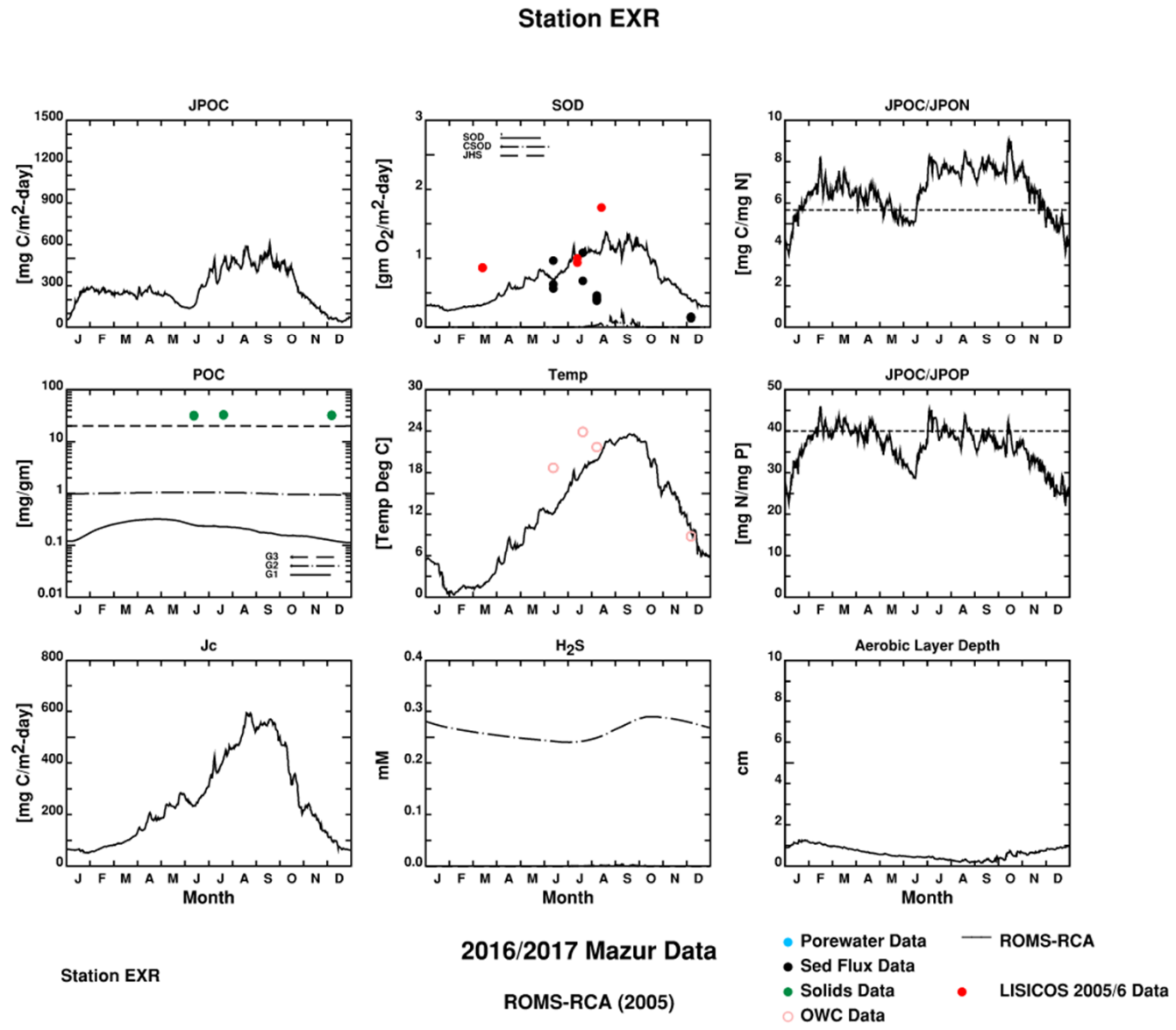
SFM FRAMEWORK

- Water quality (eutrophication) model tracks settling of phytoplankton & POM to the sediment
- It's possible that not all settling POM is incorporated into the sediment
 - Resuspension due to tides, wind events, high flow
- Water quality model uses “sticky” factor to represent what enters the sediment (VSNET)
 - VSNET assigned spatially based on sediment type



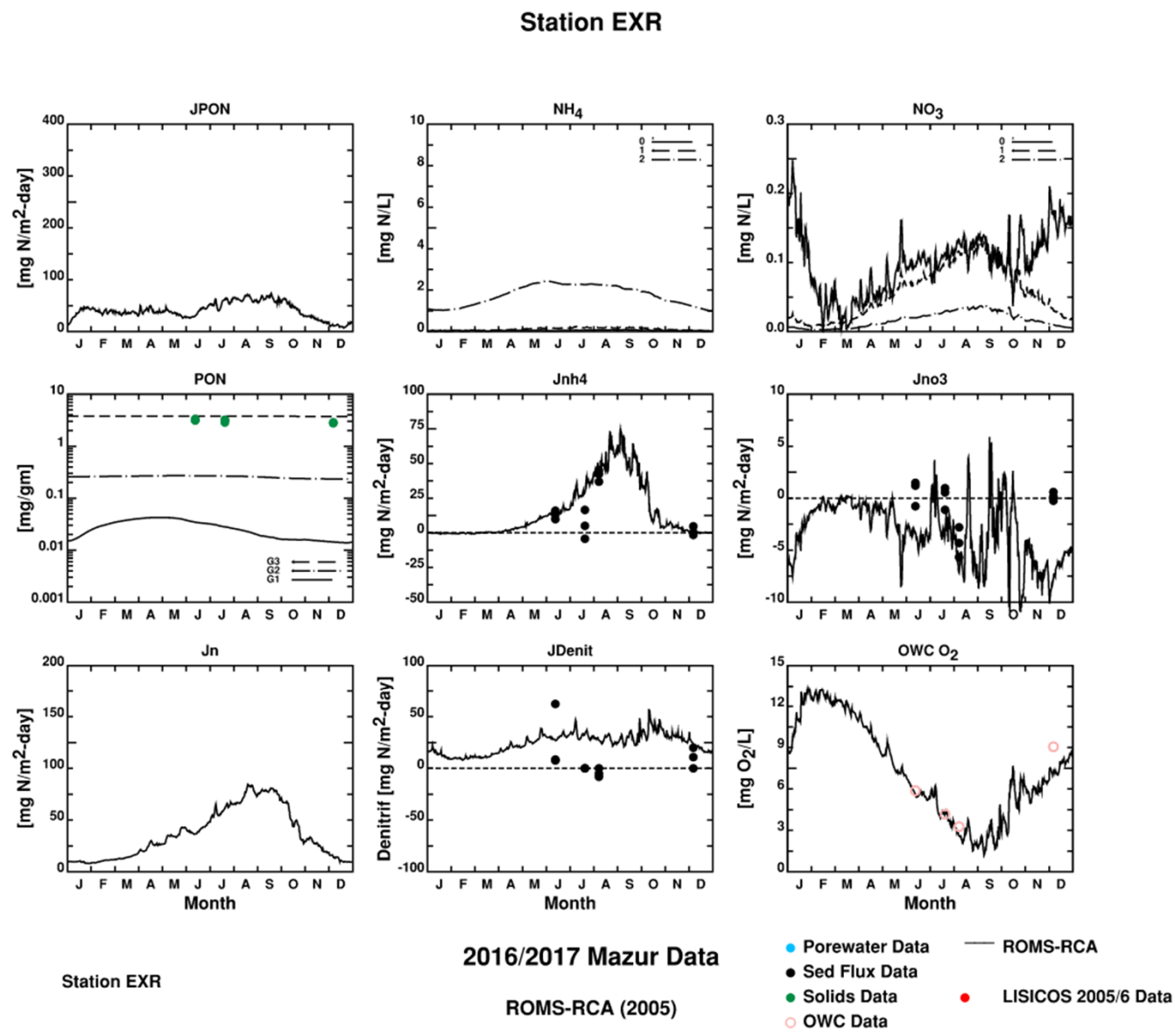
DETAILED MODEL OUTPUT

- SOD & carbon related variables



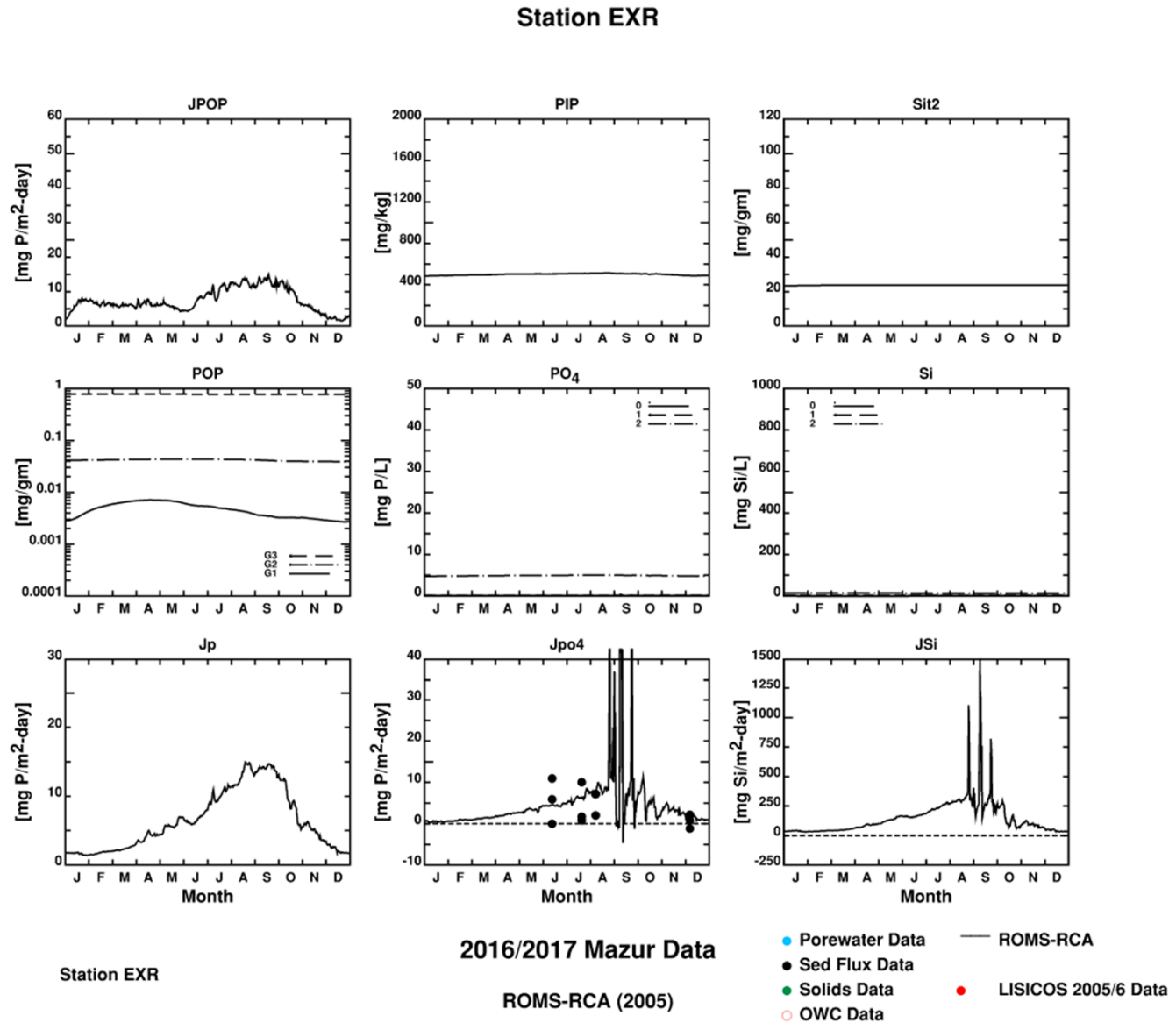
DETAILED MODEL OUTPUT

- Fluxes & nitrogen related variables



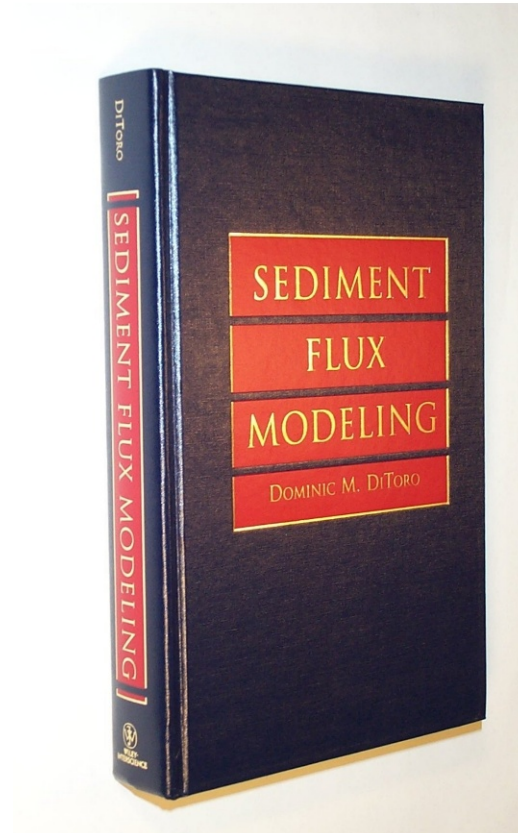
DETAILED MODEL OUTPUT

- Fluxes & phosphorus/silica related variables

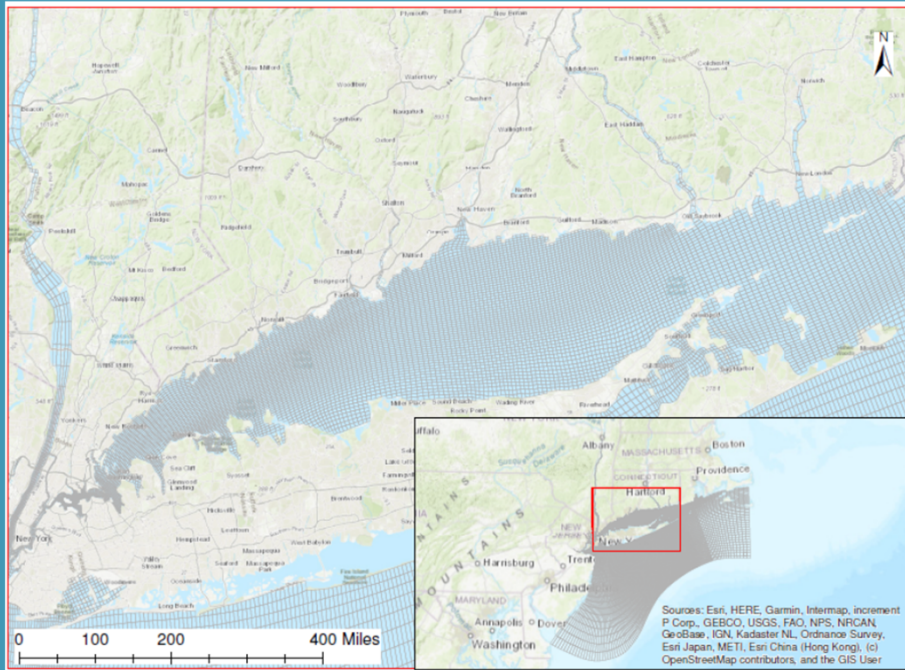


SEDIMENT FLUX MODEL

- Some light reading to understand add'l details of SFM



**Sediment Flux Modeling.
J. Wiley and Sons., 2001.
p624**



01 LIS MODEL OVERVIEW

02 ROMS HYDRODYNAMIC MODEL

03 RCA WATER QUALITY MODEL

04 **ROMS-RCA DETAILS**

ROMS-RCA CODE

- Model code in Fortran
- Running on Linux OS

Directory Structure

Compilers/	make configuration files
Data/	Input data root directory
/ROMS/	ROMS data root directory
/CDL	ROMS NetCDF metadata design
Master/	Main standalone and coupling programs
ROMS/	ROMS root directory
/Adjoint/	Adjoint model
/Biology	Adjoint biology/ecosystem models
/Bin	Executable scripts
/Drivers	Computational drivers
/External	Standard input scripts
/Functionals	Analytical expression header files
/Include	Test cases configuration header files
/Modules	Declaration modules
/Nonlinear/	Nonlinear model
/BBL	Bottom Boundary Layer formulation
RCA → /Biology	Nonlinear biology/ecosystem models
Code /SeaIce	SeaIce model
/Sediment	Nonlinear sediment transport model
/Obsolete	Discontinued files
/Programs	Support programs
/Representer/	Representer model
/Biology	Representer biology/ecosystem models
/Tangent/	Tangent linear model
/Biology	Tangent linear biology/ecosystem models
/Utility	Generic utility files
User/	ROMS User interface root directory
/External	User standard input scripts
/Functionals	User analytical expressions templates
/Include	User application header files

RCA.H BIOLOGY MODULE

▪ Clip of phytoplankton group 1 code

- Growth rate
- Growth rate reductions
- Settling
- Respiration
- Grazing/Predation

```

SYSTEM 1 - PHYT1 winter-spring diatom bloom
-----

Temperature corrected growth rate

      IF (Bio(i,k,itype).LE.TOPT(ng,1)) THEN
          GITMAX = KC(ng,1)*EXP(
&              -KBETA1(ng,1)*(Bio(i,k,itype)-TOPT(ng,1))**2.0_dp ) &
      ELSE
          GITMAX = KC(ng,1)*EXP(
&              -KBETA2(ng,1)*(TOPT(ng,1)-Bio(i,k,itype))**2.0_dp ) &
      ENDIF

Growth rate reduction due to Light attenuation

      cff1 = SKE*Hz(i,j,k)
      cff2 = ITOT/ISAT(1)
      cff_light = 2.718_dp
&              *(EXP(-cff2*EXP(-cff1))-EXP(-cff2))/cff1 &

Growth rate reduction due to nutrient limitation

&      cffN = (DNH4+Bio(i,k,iN023)) &
&              /(KMN(ng,1)+DNH4+Bio(i,k,iN023))
      cffP = DP04/(KMP(ng,1)+DP04)
      cffS = DSI/(KMS(ng,1)+DSI)
      cff_nutr = DMIN1(cffN, cffP, cffS) !MR, change from AMIN1 to DMIN1

Settling due to effect of nutrient limitation

&      ALGVS(k,1) = (VSBAS(ng,1)+VSNTR(ng,1)*(1.0_dp-cff_nutr)) &
&              *(VSBAST(ng)**TP20)

Gross growth rate of combined factors

      GPP(1) = cff_nutr*cff_light*GITMAX*Bio(i,k,iPHYT1)*P2D(i,j,iGROWTHx)

Respiration

      RESP(1) = KR6(ng,1)*GPP(1)+KRBT(ISTP20,1)*Bio(i,k,iPHYT1)

Grazing

      GRAZ(1) = 0.1*Bio(i,k,iPHYT1)*Bio(i,k,iPHYT1) !changed to 0.1* (8/21/2024)
    
```

MODEL INPUT FILES

- 14 input files required to run ROMS-RCA
- Some 2D (spatially variable)
- Some time-variable
- NetCDF and ASCII

File Name	File Description	File Type	File Size
restart.nc	Initial conditions	NetCDF	666MB
BC.nc	Boundary conditions	NetCDF	68MB
River.nc	Point source flows and loads	NetCDF	715MB
met.nc	Meteorological inputs - Wind, temperature, etc.	NetCDF	2.9GB
grd.nc	Grid file	NetCDF	6.1MB
tide.nc	Hydro tidal input	NetCDF	20MB
ATMDEP.nc	RCA atmospheric deposition	NetCDF	6.1MB
ISF.nc	RCA time-variable fraction daylight	NetCDF	16KB
ITOTSF.nc	RCA time-variable solar radiation	NetCDF	48KB
KEBSTVF.nc	RCA time-variable 2-D base light extinction coefficient	NetCDF	4.7MB
param.nc	RCA 2D and 3D parameters	NetCDF	7.1MB
rca_input.in	RCA constants and 1D parameters	ASCII	88KB
roms_input.i	Hydro constants	ASCII	156KB
stations.in	Defines the system variables and cell locations to print out in "sta" output file.	ASCII	36KB

File sizes for
1-yr simulation

RCA.IN MAIN INPUT

- ASCII/text format
- RCA related constants
- Clip of phytoplankton parameters and constants

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! STANDARD PHYTOPLANKTON DYNAMICS PARAMETERS - algal group 1 to 3
! See ID number and description in comments
!
!      GROUP1      GROUP2      GROUP3
!      -----
!
!      TOPT == 3.0d0    23.0d0    15.0d0    ! optimal growth temp. (degC)
!      KBETA1 == 0.8d-2  0.1d-1    0.8d-2    ! shaping coeff at T<=TOPT (degC^2)
!      KBETA2 == 0.1d-1  8.0d-3    8.0d-3    ! shaping coeff at T> TOPT (degC^2)
!      KC == 3.0d0      4.5d0      1.0d0      ! saturate growth rate at TOPT (1/day)
!      KT ==1.068d0     1.068d0    1.068d0    ! Arrhenius temp. coeff. growth function.
!
! New Grazing terms
!      GZTOPT == 5.0d0    25.0d0    17.0d0    ! optimal grazing temp. (degC)
!      KGZBETA1 == 7.0d-2  8.0d-2    8.0d-2    ! grazing shaping coeff at T<=GZTOPT (degC^2)
!      KGZBETA2 == 8.0d-2  8.0d-2    5.0d-2    ! grazing shaping coeff at T> GZTOPT (degC^2)
!      KGZM == 7.0d-1    7.5d-1    7.5d-1    ! grazing half-saturation PHYT C (mg C/L)
!      KRB == 0.5d-1     0.5d-1    0.5d-1    ! resting/endogenous resp. rate at 20degC (1/day)
!      KRT ==1.047d0     1.047d0    1.047d0    ! Arrhenius temperature coeff. respiration func.
!      KRG == 0.28d0     0.280d0    0.280d0    ! photosynthesis-dependent respiration coeff.
!      KIS == 125d0      250d0      125d0      ! salturation light intensity (ly/day)
!      KMN == 1.0d-2     1.0d-2     1.0d-2     ! half-saturation for nitrogen (mg N/L)
!      KMP == 1.0d-3     1.0d-3     1.0d-3     ! half-saturation for phosphorus (mg P/L)
!      KMS == 2.0d-2     2.0d-3     2.0d-2     ! half-saturation for silica (mg Si/L)
!      CCHL == 60.0d0     80.0d0     100.0d0    ! C to Chla ratio (mg C/mg Chla)
!      CPR1 == 41.0d0     41.0d0     41.0d0     ! C to P ratio non-P limited (mg C/mg P)
!      CPR2 == 90.0d0     90.0d0     90.0d0     ! C to P ratio P-limited (mg C/mg P)
!      CPR3 ==100.0d0     100.0d0     100.0d0    ! coeff. range of P-limitation (L/mg P)
!      CNR1 == 6.5d0      8.50d0     5.67d0     ! C to N ratio non-N limited (mg C/mg N)
!      CNR2 == 10.0d0     10.0d0     10.0d0     ! C to N ratio N-limited (mg C/mg N)
!      CNR3 == 15.0d0     15.0d0     15.0d0     ! coeff. range of N-limitation (L/mg N)
!      CSR1 == 2.0d0      7.0d0      3.0d0      ! C to Si ratio non-Si limited (mg C/mg Si)
!      CSR2 == 10.0d0     10.0d0     10.0d0     ! C to Si ratio Si-limited (mg C/mg Si)
!      CSR3 == 30.0d0     30.0d0     30.0d0     ! coeff. range of Si limitation (L/mg Si)
!      XKC == 1.7d-2     1.7d-2     1.7d-2     ! chl self-shading extinction coeff (m^2/mg Chla)
!      VSBAS == 0.3d0     2.0d-1     0.5d0      ! base algal settling rate (m/day)
!      VSNTR == 0.5d0     0.6d0      0.3d0      ! nutrient stressed algal setting rate (m/day)
!      KMPHYT == 0.25d0                                ! phytoplankton half saturation (mg C/L)
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ROMS-RCA OUTPUT FILES

- roms_rst.nc (666MB) – “restart” file, initial conditions for hot-starting (water column & sediment)
- roms_his.nc (5.5GB) – instantaneous time-series output at all model cells
- roms_sta.nc (225MB) – instantaneous time-series output at pre-determined list of model cells, for high-frequent time-series output
- log (76MB) – text file, updates in real-time, good for debugging/diagnostics
- File sizes for a 30-day output block
 - Output frequency: roms_his.nc = 12hr, roms_sta.nc = 1hr

ROMS-RCA RUNTIME

- Tiling = 8x4, 32 CPU (for parallel processing)
- Model grid = 307 x 143 x 10
- Total water segments = 184,490

- ROMS (hydro only): @ 5 sec timestep = 24 hrs simulation time/model year
- ROMS-RCA (hydro + WQ): @ 6 sec timestep = 50 hrs simulation time/model year

