Appendix E: State Variable Calculation

1. Problem Statement

Boundary flows include ocean boundaries, tributaries, runoff, treated wastewater, and combined sewer overflows. For every boundary flow, concentrations must be assigned for each state variable simulated in the water quality model. The state variables simulated in the water quality model are shown below.

Dissolved Constituents	**Particulate Constituents**
Inorganic nutrients	Phytoplankton Biomass
NH-34: ammonia nitrogen	PHYTO1: spring marine diatom community
NO3O2: nitrate(+nitrite) nitrogen	PHYTO2: summer freshwater diatom community
D-DIP: inorganic phosphate	PHYTO3: summer marine diatom community
IN-SI: inorganic silica	
	Detritus
Organic nutrients	DET-C: detrital carbon
CBODU1: ultimate CBOD from stream	DET-N: detrital nitrogen
CBODU2: ultimate CBOD from PS	DET-P: detrital phosphorus
CBODU3: refractory CBOD	DET-SI: detrital silica
ORG-N: dissolved organic nitrogen	
ORG-P: dissolved organic phosphorus	
ORG-SI: dissolved organic silica	
Gases	
DISOX: dissolved oxygen	

A few of these state variables, such as dissolved oxygen, are measured directly. State variable concentrations were calculated based on measured data in order to develop boundary conditions, such as tributaries and treatment plant discharges, and to prepare model-data comparisons. Methodologies and assumptions used for these calculations are documented herein.

2. NITROGEN COMPONENTS

State variables associated with nitrogen are listed below.

- NH34: ammonia nitrogen
- NO3O2: nitrate + nitrite nitrogen
- ORG-N: dissolved organic nitrogen
- DET-N: detrital nitrogen
- Phyto: phytoplankton (modeled as carbon with Nitrogen-to-Carbon ratio)

Datasets used to prepare boundary conditions and calibration data include the analytical parameters relevant to nitrogen listed below.

- Filtered and unfiltered
    - NH_3: ammonia, as N
    - NO_3: nitrate, as N
    - NO_2+NO_3: nitrate + nitrite, as N
- Filtered
    - SKN: soluble Kjeldahl nitrogen
    - DON: dissolved organic nitrogen
    - TDN: total dissolved nitrogen
- Unfiltered
    - TKN: total Kjeldahl nitrogen
    - TN: total nitrogen
    - TSN: total suspended nitrogen

In this study, state variables associated with nitrogen are calculated using the equations shown below in order of preference based on available measured data. Negative values for components were set to zero or a nominal non-zero value.

- Ammonia nitrogen
    - NH34 ≈ NH_3 (filtered if available, otherwise unfiltered)
- Nitrate nitrogen
    - NO3O2 ≈ NO_2+NO_3 (filtered then unfiltered); or
    - NO3O2 ≈ NO_3 (filtered then unfiltered)

- Dissolved organic nitrogen
  - ORG-N ≈ DON; or
  - ORG-N ≈ (SKN – NH34); or
  - ORG-N ≈ (TDN – NH34 – NO3O2); or
  - ORG-N ≈ (TN – TSN – NH34 – NO3O2); or
  - ORG-N ≈ f_{Ndiss} * (TKN – NH34)
- Detrital nitrogen
  - DET-N ≈ (TKN – SKN) – r_{na}* Chla; or
  - DET-N ≈ TSN – r_{na} * Chla; or
  - DET-N ≈ (TN – TDN) – r_{na}* Chla; or
  - DET-N ≈ (1-f_{Ndiss}) * (TKN – NH34) – r_{na}* Chla

where:

- r_{na} = 7.434×10^{-3} mgN/µgChla in phytoplankton (Chapra 1997 and Chapra et al., 2012)
- f_{Ndiss} = fraction of dissolved portion in total organic nitrogen (assumed)
  - 0.50 for all tributaries and ocean
  - 0.75 for municipal WWTPs
  - 0.50 for industrial WWTPs

3. PHOSPHORUS COMPONENTS

State variables associated with phosphorus are listed below.

- D-DIP: inorganic phosphate
- ORG-P: dissolved organic phosphorus
- DET-P: detrital phosphorus
- Phyto: phytoplankton (modeled as carbon with Phosphorus-to-Carbon ratio)

Datasets used to prepare boundary conditions and calibration data include the analytical parameters relevant to phosphorus listed below.

- Filtered
  - PO_4: orthophosphate (also unfiltered)
  - TDP: total dissolved phosphorus
  - DAHP: dissolved acid-hydrolizable P
- Unfiltered
  - TP: total phosphorus

- AHP: acid-hydrolizable phosphorus

In this study, state variables associated with phosphorus are calculated using the equations shown below in order of preference based on available measured data. Negative values for components were set to zero or a nominal non-zero value.

- Dissolved inorganic phosphate
  - D-DIP ≈ PO4; or
  - D-DIP ≈ TDP; or
  - D-DIP ≈ DAHP; or
  - D-DIP ≈ AHP
- Dissolved organic phosphorus
  - ORG-P ≈ TDP – D-DIP; or
  - ORG-P ≈ f_{Pdiss} * (TP – D-DIP – r_{pa}* Chla)
- Detrital phosphorus
  - DET-P = (TP - TDP) – r_{pa}* Chla; or
  - DET-P ≈ (1- f_{Pdiss}) * (TP – D-DIP – r_{pa}* Chla)
- If only TP is available
  - D-DIP ≈ f_{Pinorg}* TP
  - ORG-P ≈ f_{Pdiss} * (1-f_{Pinorg}) * TP
  - DET-P ≈ (1- f_{Pdiss}) * (1-f_{Pinorg}) * TP

where:

- r_{pa} = 9.24×10^{-4} mgP/µgChla in phytoplankton (Chapra 1997 and Chapra et al., 2012)
- f_{Pdiss} = fraction of dissolved portion in total organic phosphorous = 0.1 (assumed)
- f_{Pinorg} = fraction of inorganic portion in total phosphorous (assumed)
  - 0.1 for ocean
  - 0.5 for tributaries
  - 0.9 for WWTPs

4. CARBON COMPONENTS

State variables associated with carbon are listed below.

- CBODU: carbonaceous biological oxygen demand ultimate (mg-O2/L)
  - CBODUTrib: tributaries
  - CBODUPS: treatment plants

    - CDOM: refractory portion
- DET-C: detrital carbon
- Phyto: phytoplankton (µg/L as chla)

Datasets used to prepare boundary conditions and calibration data include the analytical parameters relevant to carbon listed below.

- Filtered
    - DOC: dissolved organic carbon
- Unfiltered
    - $CBOD_5$: 5-day CBOD
    - TOC: total organic carbon
    - $CBOD_{20}$: 20-day CBOD (ceased in 2019)
    - COD: chemical oxygen demand
    - BOD_{90}: 90-day biochemical oxygen demand (2 studies: tribs, WWTPs)

In this study, state variables associated with carbon are calculated using the equations shown below in order of preference based on available measured data. Negative values for components were set to zero or a nominal non-zero value.

- If DOC and TOC are available
    - $CBODU \approx 2.67 * DOC * [1–f_{Crefr}]$
    - $CDOM \approx 2.67 * DOC * f_{Crefr}$
    - $DET\text{-}C \approx TOC – DOC – r_{ca} * Chla$
- If only TOC is available:
    - $CBODU \approx 2.67 * TOC * f_{Cdiss} * [1–f_{Crefr}]$
    - $CDOM \approx 2.67 * TOC * f_{Cdiss} * f_{Crefr}$
    - $DET\text{-}C \approx TOC * (1–f_{Cdiss}) – r_{ca} * Chla$
- If only CBOD5 is available:
    - $CBODU \approx [CBOD_5/(1–EXP(-k1*5))] * f_{Cdiss}$
    - $CDOM \approx [CBODU/(1–f_{Crefr})] * f_{Crefr}$
    - $DET\text{-}C \approx (CBOD_5/2.67)/(1–EXP(-k1*5)) * (1–f_{Cdiss}) – r_{ca} * Chla$

where:

- f_{Crefr} = fraction of refractory portion in total organic carbon (based on BOD_{90} studies)
    - 0.74 For Delaware River at Trenton
    - 0.88 for Rancocas Creek (north and south branches)
    - 0.69 for all other tributaries

  - 0.70 for ocean (including C&D Canal)
  - 0.65 from industrial WWTPs
  - 0.50/0.40 from Tier 1 WWTPs in summer/winter
  - 0.40/0.35 from Tiers 2 and 3 in summer/winter
- f_{Cdiss} = fraction of dissolved portion in total organic carbon
  - DOC/TOC ratio calculated for each facility/tributary; OR
  - 0.98 (assumed)
- r_{ca} = 0.042 mgC/µgChla in phytoplankton (Chapra 1997 and Chapra et al., 2012)
  - Chla assumed to be zero for all wastewater.
- k1 = CBOD decay rate (estimated from BOD_{90} studies)
  - 0.087/day for wastewater CBOD
  - 0.033/day for tributaries

5. SILICA COMPONENTS

State variables associated with silica are listed below.

- IN-Si: inorganic silica
- ORG-Si: dissolved organic silica
- DET-Si: detrital silica
- Phyto: phytoplankton (modeled as Carbon with Silica-to-Carbon ratio)

Datasets used to prepare boundary conditions and calibration data include the analytical parameters relevant to silica listed below.

- Filtered
  - DSi: dissolved silica
- Unfiltered
  - TSi: total silica
  - BSi: biogenic silica (SiO2)

In this study, state variables associated with silica are calculated using the equations shown below in order of preference based on available measured data. Negative values for components were set to zero or a nominal non-zero value.

- If TSi or BSi is available in addition to DSi:
  - IN-Si ≈ DSi
  - DET-Si ≈ (1- f_{Sdiss}) * BSi – r_{sa}* Chla
  - ORG-Si ≈ f_{Sdiss} * BSi

    - If BSi is not available, substitute with (TSi – DSi)
- If only DSi is available:
    - IN-SI ≈ DSi
    - DET-Si ≈ (1- f_{Sdiss}) * (DSi/$f_{Silnorg}$– DSi) – r_{sa}* Chla
    - ORG-Si ≈ f_{Sdiss} * (DSi/$f_{Silnorg}$– DSi)

where:

Based on Barnegat system median DSi/TSi ratios (Zafer et al. 2017):

    - $f_{Silnorg}$ = 0.98 for tributaries; and
    - $f_{Silnorg}$ = 0.53 for ocean (and C&D Canal)
- f_{Sdiss} = fraction of dissolved portion in total organic silica = 0.05 (assumed)
- r_{sa} = 8.4×10^{-3} mgSi/µgChla in phytoplankton (Reference)

Assumptions/Methodology related to silica components

- DSi is equal to dissolved inorganic silica (all inorganic silica is dissolved).
- BSi includes all forms of organic silica: DetritalSi, PhytoSi, and Dissolved. While the BSi test only measures particulate matter, we are still going to take the dissolved organic fraction out of this box.
- In theory, TSi should equal DSi plus BSi (Barnegat data bear this out).
- We can assume that 5% of the organic silica is dissolved, leaving the other 95% in PhytoSi or DetSi. This 5% value is consistent with the ratio of BSi to Psi observed in the Barnegat Bay boundaries.
- Use river/tributary data to estimate PS Silica concentrations.

6. SUSPENDED SOLIDS

State variables associated with suspended solids are listed below.

- Organic Solids
    - POM (particulate organic material)
        - C, N, P, Si and D (Dry Weight)
    - Phytoplankton biomass
        - As C
        - N, P, Si and D by stoichiometry
- Inorganic Solids
    - ISS: inorganic suspended solids

Relevant analytical parameters measured by agencies and NPDES permit-holders contain:

- Total solids (TS)
- Total suspended solids (TSS)
- Total volatile solids (TVS)
- Total fixed solids: TS minus TVS
- Volatile suspended solids (VSS)

In this study, state variables associated with suspended solids are calculated as below:

- If VSS is available
    - ISS = TSS – VSS
- If TVS is available
    - ISS = TSS * (1 – TVS/TS)
- If no volatile solids measurements
    - ISS = TSS * f_{Sinorg}

where:

- f_{Sinorg} = fraction of ISS portion in TSS
    - median (1 – TVS/TS) for tributaries and ocean
    - 0.15 for treated wastewater (assumed)