Appendix K. Verification Tests for GEMSS

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GEMSS Verification Tests

Recommended Tests for Data Input and Process Algorithms

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This report documents a set of tests to verify the implementation of water quality algorithms in GEMSS modules WQCBM, GAM (i.e., GenAlgae), and WQADD. These tests were compiled during late July and early August 2010.

Approach

The model verification tests described here use the general strategy of simplifying the model domain and data input drastically in order to isolate individual algorithms or groups of algorithms with known solutions. Most water quality equations are based on mass balance and first-order kinetics which, after input parameter adjustments, produce specific half-lives or doubling times. Analytical solutions, then, are developed for half lives of 1, 2, 5, and 10 days and doubling times of 1 and 2 days. Model parameters are specified to produce reaction rate constants with these specific half lives.

The verification tests are designed to assure that the model correctly executes the following:

- Delivery of input data to model algorithms
- Manipulation of data, including units conversions
- Solution of water quality process equations to acceptable accuracy
- Delivery of calculated data to output variables

These tests are not designed to check for protection against user error, including the input of extreme data that are out of the range of the model algorithms. Those can often be checked by deliberately providing bad input data and noting the model's response.

These tests do not address model conception errors, which might be introduced, for example, by representing a complex set of water quality reactions using a single lumped parameter equation or by representing a water quality reaction using a complex equation with several unknown parameters that cannot be measured.

Summary

Two types of tests are described here. The first type tests overall mass balances as water quality variable cycle through sets of reactions. Five specific tests are described. The second type tests specific water quality reactions for accurate kinetics. Twenty specific tests are described, most of which require multiple model runs for three water temperatures and other varying initial or environmental conditions.

Water Quality Mass Balance Tests

This series of test simulations verifies that water quality mass balances are maintained. Specific values for cell volume are not important in these tests. For consistency, a cell volume of 10,000 m^3 is recommended.

Specific rate constants and kinetic coefficients are not important in these tests. For consistency, the following environmental conditions and kinetic coefficients are recommended for these tests:

- Light saturation constant: 100 W/m^2 (or 200 Ly/day)
- Optimum temperature for growth: 20 C
- Half-saturation constant for N limitation: 0.01 mg/L
- Half-saturation constant for P limitation: 0.002 mg/L
- Maximum growth rate constant: 2.5 day^{-1}
- Respiration rate constant: 0.1 day^{-1}
- Death rate constant: 0.05 day^{-1}
- Grazing rate constant: 0.05 day^{-1}
- Fraction of phytoplankton death going to CBOD: 0.4
- Fraction of phytoplankton CBOD source allocated to fast CBOD: 0.5
- Excretion fraction: 0.01
- Detrital dissolution rate constant: 0.1 day^{-1}
- Organic matter mineralization rate constants: 0.1 day^{-1}
- Nitrification rate constant: 0.1 day^{-1}
- Denitrification rate constant: 0
- Reaeration rate constant: 0.5 day^{-1}
- Settling rates or velocities: 0
- Temperature correction coefficients ("theta"): 1.08
- CBOD decay rate constants: 0

To obtain the proper phytoplankton N and P concentrations, set the following initial phytoplankton compositional ratios:

- D:C ratio: 2
- N:C ratio: 0.2
- P:C ratio: 0.05
- Chl:C ratio: 0.02 (i.e., C:Chl = 50)

Other variables and forcing functions should be set to levels that do not inhibit nutrient cycling. Recommended values are:

- Dissolved oxygen: 10 mg/L
- Water temperature: 20 C
- Inorganic solids: 10 mg/L
- Incident light: 250 W/m^2 (or 500 Ly/day)
- Fraction PAR: 50%
- Fraction daylight: 0.5

If possible, bypass the DO simulation so that oxygen levels remain high. Run the simulation for duration equal to 10 half-lives of the slowest reaction.

Test 1.1 – Total Nutrient Concentrations in CSTR with No Flow

In a static system with no loss reactions, nitrogen and phosphorus should cycle among organic and inorganic species while maintaining their initial overall concentrations. This tests the maintenance of mass balance in the nutrient cycling algorithms.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. The specific values of initial concentrations and rate constants do not matter much for this test. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

Set initial concentrations so that TN is 1 mg/L and TP is 0.4 mg/L. Recommended initial species concentrations are:

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- NH_4: 0.5 mg/L
- NO_3: 0.1 mg/L
- Detrital N: 0.1 mg/L
- Dissolved organic N: 0.1 mg/L
- PO4: 0.25 mg/L
- Detrital P: 0.05 mg/L
- Dissolved organic P: 0.05 mg/L

Run the simulation for a duration of 10 years to test for absence of long-term numerical drift. Check TN and TP for stable concentrations of 1 mg/L and 0.4 mg/L, respectively.

Test 1.2 – Total Nutrient Concentrations in CSTR with Flow

In a flow-through system with no loss reactions, nitrogen and phosphorus should cycle among organic and inorganic species while converging to and then maintaining a steady-state distribution where ambient TN and TP concentrations equal boundary TN and TP concentrations. This tests the overall mass balance of the nutrient cycles.

To conduct these tests, set initial concentrations, dispersion coefficients and settling velocities to 0. Set the advective flow to a steady value so that the hydraulic residence time (volume/flow) is several days. Recommended values for volume and flow are 10,000 m^3 and 2000 m^3/day (0.02315 m^3/sec), respectively.

The specific boundary concentrations and rate constants do not matter much for this test. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

Set boundary concentrations so that TN is 1 mg/L and TP is 0.4 mg/L. Recommended boundary concentrations are:

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- NH_4: 0.5 mg/L
- NO_3: 0.1 mg/L
- Detrital N: 0.1 mg/L
- Dissolved organic N: 0.1 mg/L
- PO_4: 0.25 mg/L
- Detrital P: 0.05 mg/L
- Dissolved organic P: 0.05 mg/L

Run the simulation for a duration of 10 years to test for absence of long-term numerical drift. Check TN and TP for stable concentrations of 1 mg/L and 0.4 mg/L, respectively.

Test 1.3 – Phytoplankton to Inorganic Nutrient Pathway in CSTR with No Flow

In a static system with no growth and no loss reactions, phytoplankton nitrogen and phosphorus should cycle through detritus and dissolved organic matter and accumulate as NO_3 and PO_4 while maintaining their initial TN and TP concentrations. With no refractory POC fraction and no CBOD decay, phytoplankton carbon should produce a fraction of CBOD equal to the death plus grazing rates divided by the respiration plus death plus grazing rates (adjusted by the stoichiometric ratio of 32/12 gO_2/gC). This tests mass balance pathways for the carbon and nutrient cycles.

In WQCBM, phytoplankton excretion and a fraction of death, *foc*×*fd5*, are sources of fast-reacting CBOD. Slow-reacting CBOD receives a complimentary fraction of phytoplankton death, *foc*×*(1-fd5)*. The remaining fraction of phytoplankton death, *1-foc*, and phytoplankton grazing is directed to detrital C; if refractory POC pathways *fd9r* and *fg9r* are set to 0, this carbon eventually cycles to slow-reacting CBOD. Since growth and thus excretion is 0, the final fast and slow CBOD concentrations should increase by:

$$\Delta CBOD_f = PhytC\left(\frac{32}{12}\right)\frac{foc\times fd5\times k_D}{k_R + k_D + k_G}$$

$$\Delta CBOD_s = PhytC\left(\frac{32}{12}\right)\frac{(1-foc\times fd5)k_D + k_G}{k_R + k_D + k_G}$$

In these tests, rate constants for respiration, death, and grazing are set to 0.1, 0.05, and 0.05 day^{-1}, respectively. With initial CBOD concentrations set to 0, *foc* set to 0.4 and *fd5* set to 0.5, the final carbon fractions in CBOD_f and CBOD_s should be 0.01/0.2, or 0.05, and 0.09/0.2, or 0.45. The final CBOD_f and CBOD_s concentrations should be 0.13333 and 1.2 mgO_2/L, respectively.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that denitrification and CBOD deoxygenation reactions are set to 0. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

Set the following initial concentrations:

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- NH_4: 0 mg/L
- NO_3: 0 mg/L
- Detrital N: 0 mg/L
- Dissolved organic N: 0 mg/L
- PO_4: 0 mg/L
- Detrital P: 0 mg/L
- Dissolved organic P: 0 mg/L
- $CBOD_f$: 0 mg/L
- $CBOD_s$: 0 mg/L

Run the simulation for duration equal to 10 half-lives of the slowest reaction. Here, the death rate constant is 0.05 day-1, giving a half life of about 14 days, so the simulation should run for 140 days. Check TN and TP for stable concentrations of 0.2 mg/L and 0.05 mg/L, respectively, and check final NO_3 and PO_4 concentrations for these same values. Check final $CBOD_f$ and $CBOD_s$ concentrations for values of 0.13333 mg/L and 1.2 mg/L, respectively.

Test 1.4a – WQCBM Phytoplankton to Inorganic Carbon Pathway in CSTR with No Flow

In a static system with no growth and no loss reactions, phytoplankton carbon should cycle through detritus and dissolved organic matter and accumulate as refractory POC and inorganic carbon (TIOC) while maintaining its initial total carbon concentration. This tests mass balance pathways for the carbon cycle using the organic carbon-CBOD pathways in WQCBM.

The WQCBM carbon cycle is illustrated in Figure 1. Note that TIOC is simulated in WQADD.

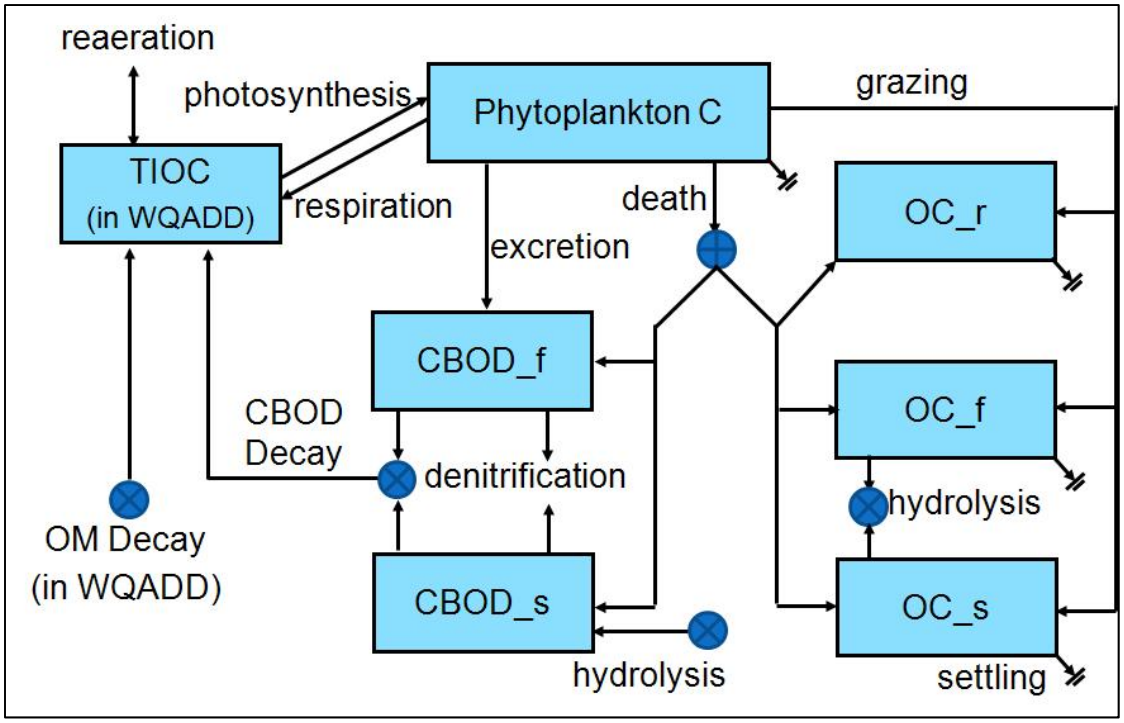

Figure 1 - WQCBM Carbon Cycle

In WQCBM, a fraction of death, (1-*foc)*×*fd9r*, and a fraction of grazing, *fg9r*, are sources of refractory POC. The remaining fractions of phytoplankton death and grazing are directed to CBOD and reactive POC, and eventually cycle to TIOC. Phytoplankton respiration is a direct source of TIOC. Since growth and thus excretion is 0, the ultimate change in OC_r and TIOC concentrations should be:

$$\Delta OC_r = PhytC \times \frac{(1-foc)fd9r \times k_D + fg9r \times k_G}{k_R + k_D + k_G}$$

$$\Delta TIOC = PhytC \times \frac{k_R + (1 + foc \times fd9r - fd9r) \times k_D + (1 - fg9r) \times k_G}{k_R + k_D + k_G}$$

In these tests, rate constants for respiration, death, and grazing are set to 0.1, 0.05, and 0.05 day^{-1}, respectively. With *foc* set to 0.4, *fd9r* set to 0.2, and *fg9r* set to 0.6, OC_r should increase by 0.036/0.2, or 0.18 mg/L, and TIOC should increase by 0.164/0.2, or 0.82 mg/L.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that the phytoplankton growth and WQADD organic matter reactions (particularly decay) are set to 0, and that reaeration rate constant is 0. The following rate constants and coefficients should be assigned:

- Phytoplankton growth rate constant: 0 day^{-1}
- Phytoplankton respiration rate constant: 0.1 day^{-1}

- Phytoplankton death rate constant: 0.05 day^{-1}
- Phytoplankton grazing rate constant: 0.05 day^{-1}
- Fraction phytoplankton death to CBOD pathway: 0.4
- Fraction of phytoplankton CBOD death pathway to CBOD_f: 0.5
- Fraction of phytoplankton POC death pathway to OC_f: 0.4
- Fraction of phytoplankton POC death pathway to OC_s: 0.4
- Fraction of phytoplankton POC death pathway to OC_r: 0.2
- Fraction of phytoplankton grazing pathway to OC_f: 0.2
- Fraction of phytoplankton grazing pathway to OC_s: 0.2
- Fraction of phytoplankton grazing pathway to OC_r: 0.6
- OC_f hydrolysis rate constant: 0.1 day^{-1}
- OC_s hydrolysis rate constant: 0.05 day^{-1}
- CBOD decay rate constants: 0.1 day^{-1}`
- LPOM dissolution rate constant: 0 day^{-1}
- RPOM dissolution rate constant: 0 day^{-1}
- LDOM decay rate constant: 0 day^{-1}
- RDOM decay rate constant: 0 day^{-1}
- LPOM decay rate constant: 0 day^{-1}
- RPOM decay rate constant: 0 day^{-1}
- LDOM transformation rate constant: 0 day^{-1}
- LPOM transformation rate constant: 0 day^{-1}
- Reaeration rate constant: 0 day^{-1}

Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups. Set the following initial concentrations:

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- NH_4: 0 mg/L
- NO_3: 0 mg/L
- Detrital N: 0 mg/L
- Dissolved organic N: 0 mg/L
- PO_4: 0 mg/L
- Detrital P: 0 mg/L
- Dissolved organic P: 0 mg/L
- $CBOD_f$: 0 mg/L
- $CBOD_s$: 0 mg/L
- TIOC: 0 mg/L

If initial TIOC cannot be specified or run separately from pH and alkalinity, then set initial pH to 7.7 and alkalinity to 100 mg $CaCO_3$/L. With a temperature of 20 C and salinity of 0 PSU, the corresponding initial TIOC concentration should be 24.891 mg/L.

Run the simulation for duration equal to 10 half-lives of the slowest reaction. Here, the death rate constant is 0.05 day-1, giving a half life of about 14 days, so the simulation should run for 140 days. Check total carbon for a stable concentration of either 1.0 mg/L or 25.891 mg/L (depending on the initial TIOC concentration). Check the final OC_R concentration for a value of 0.18 mg/L. Check the final TIOC concentration for an increase of 0.82 mg/L to either 0.82 mg/L or 25.711 mg/L.

Test 1.4b – WQADD Phytoplankton to Inorganic Carbon Pathway in CSTR with No Flow

In a static system with no growth and no loss reactions, phytoplankton carbon should cycle through detritus and dissolved organic matter and accumulate as inorganic carbon (TIOC) while maintaining its initial total carbon concentration. This tests mass balance pathways for the carbon cycle using the organic matter pathways in WQADD.

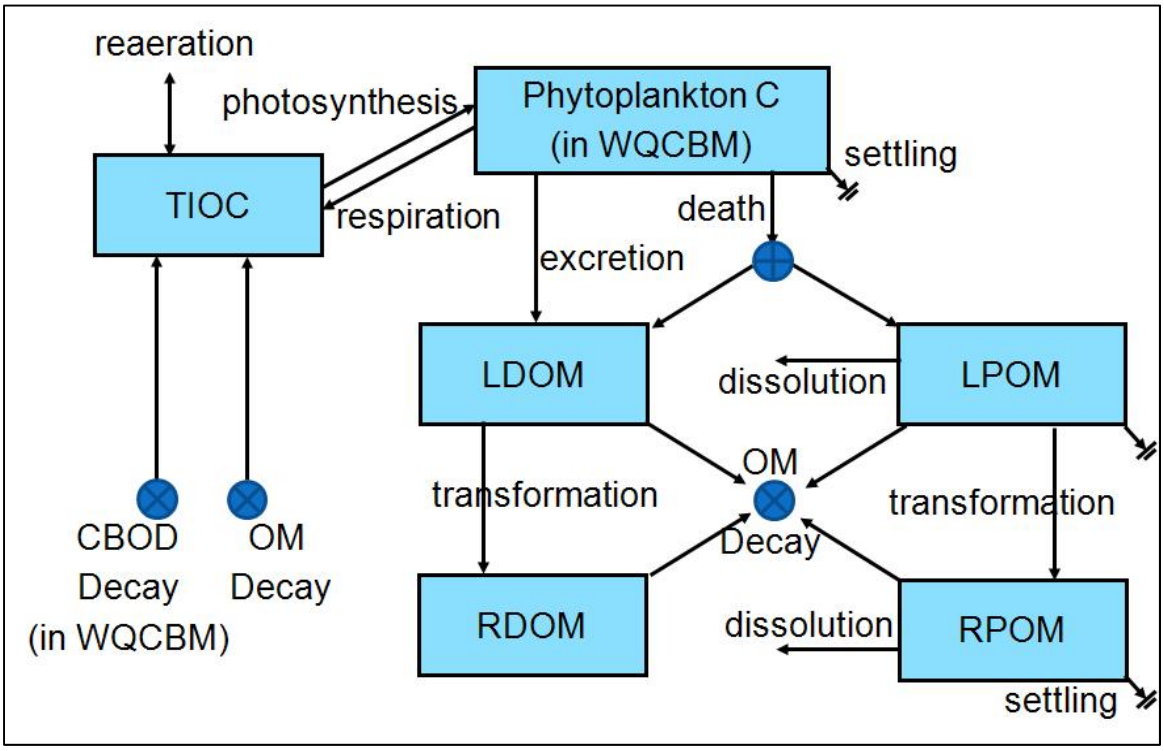

Figure 2 - WQADD Carbon Cycle

The WQADD carbon cycle is illustrated in Figure 2. Note that Phytoplankton is simulated in WQCBM.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that the WQCBM phytoplankton growth and CBOD decay and the WQADD dissolution reactions are set to 0, and that reaeration rate constant is set to 0. The following rate constants and coefficients should be assigned:

- Phytoplankton growth rate constant: 0 day^{-1}

- Phytoplankton grazing rate constant: 0 day^{-1}
- Fraction of phytoplankton death pathway to LPOM: 0.6
- CBOD decay rate constants: 0 day^{-1}`
- LPOM dissolution rate constant: 0 day^{-1}
- RPOM dissolution rate constant: 0 day^{-1}
- LDOM decay rate constant: 0.1 day^{-1}
- RDOM decay rate constant: 0.02 day^{-1}
- LPOM decay rate constant: 0.1 day^{-1}
- RPOM decay rate constant: 0.02 day^{-1}
- LDOM transformation rate constant: 0.1 day^{-1}
- LPOM transformation rate constant: 0.1 day^{-1}
- Reaeration rate constant: 0 day^{-1}

Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups. Set the following initial concentrations:

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- NH_4: 0 mg/L
- NO_3: 0 mg/L
- Detrital N: 0 mg/L
- Dissolved organic N: 0 mg/L
- PO_4: 0 mg/L
- Detrital P: 0 mg/L
- Dissolved organic P: 0 mg/L
- $CBOD_f$: 0 mg/L
- $CBOD_s$: 0 mg/L
- LDOM: 0 mg/L
- RDOM: 0 mg/L
- LPOM: 0 mg/L
- RPOM: 0 mg/L
- TIOC: 0 mg/L
- Or, pH 7.7, alkalinity 100 mg/L, TIOC 24.891 mg/L

Run the simulation for duration equal to 10 half-lives of the slowest reaction. Here, the RDOM decay rate constant is 0.02 day-1, giving a half life of about 35 days, so the simulation should run for 350 days. Check total carbon for a stable concentration of either 1.0 mg/L or 25.891 mg/L (depending on the initial TIOC concentration) and check final TIOC concentration for this same value.

Test 1.5 – Detritus to Phytoplankton Nutrient Pathway in CSTR with No Flow

In a static system with phytoplankton growth with no excretion, respiration, or death, detrital N and P should cycle through dissolved organic matter, inorganic N and P, and accumulate as phytoplankton N and P while maintaining the initial TN and TP concentrations. This tests mass balance pathways for the nutrient cycles.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that denitrification is set to 0. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

Set the initial concentrations so that TN and TP are 0.2 mg/L and 0.05 mg/L respectively:

- Phytoplankton C: 0.01 mg/L
- Phytoplankton N: 0.002 mg/L
- Phytoplankton P: 0.0005 mg/L
- NH_4: 0 mg/L
- NO_3: 0 mg/L
- Detrital N: 0.188 mg/L
- Dissolved organic N: 0 mg/L
- PO_4: 0 mg/L
- Detrital P: 0.0495 mg/L
- Dissolved organic P: 0 mg/L

Run the simulation for duration equal to 10 half-lives of the slowest reaction. For a limiting reaction rate constant of 0.1 day^{-1}, the half life is about 7 days, so the simulation should run for 70 days. Check TN and TP for stable concentrations of 0.2 mg/L and 0.05 mg/L, respectively, and check final phytoplankton N and P concentrations for these same values. Final phytoplankton C should approach 1.0 mg/L (because half-saturation constants will limit growth, the final phytoplankton C, N and P should be over 0.99 mg/L, 0.19 mg/L, and 0.049, respectively.

Water Quality Kinetics Tests

This series of test simulations verifies that water quality kinetic reactions are implemented correctly, that input coefficients are transferred properly, and that the numerical solution is accurate. Specific values for cell volume are not important in these tests. For consistency, a cell volume of 10,000 m^3 is recommended.

Most water quality reactions are implemented as first-order transformations:

$$C_R \xrightarrow{k} a\,C_P$$

where C_R is reactant concentration, mg/L, C_P is product concentration, mg/L, k is first-order decay rate constant, day^{-1}, and a is the stoichiometric ratio, g_P/g_R.

$$\frac{dC_R}{dt} = -k C_R$$

In these reactions, decay of the reactant transfers mass to the product:

$$\frac{dC_P}{dt} = k a C_R$$

For growth reactions, k is first-order growth rate constant, day^{-1}:

$$\frac{dC_P}{dt} = k C_P$$

In these reactions, growth of the product draws down mass from the reactant.

Although the water quality verification tests described here can be conducted with a range of rate constants and kinetic coefficients, it is convenient to specify values that result in half lives of 1, 2, 5, or 10 days. For first-order kinetics, half-life $t_{½}$ is related to rate constant k by:

$$t_{1/2} = \frac{-\ln(0.5)}{k} = \frac{0.6931472}{k}$$

Similarly, doubling time for first-order growth reactions is related to rate constant k by:

$$t_2 = \frac{\ln(2)}{k} = \frac{0.6931472}{k}$$

Most water quality reactions are adjusted for water temperature using the "theta" temperature correction approach:

$$k = k_{20} \cdot \theta^{T-20}$$

Where k_{20} is the reaction rate constant at 20C, θ is the temperature correction factor, and T is water temperature. For θ of 1.08, the values of k_{20} (to 6 significant figures) that produce selected half-lives at three water temperatures are given in Table 1.

Table 1 - Reaction rate constants for select half-lives

	Reaction Half Life or Doubling Time			
Temperature	1 day	2 days	5 days	10 days
10 C	1.496453	0.748226	0.299291	0.149645
20 C	0.693147	0.346574	0.138629	0.0693147
30 C	0.321061	0.160531	0.0642123	0.0321061

In the following tests, the water temperature and reaction rate constant k_{20} should be input, along with temperature correction factor of 1.08.

For some water quality reactions as noted below, additional kinetic constants and environmental properties must be specified to obtain the desired k_{20} values. Initial reactant and product concentrations should be set to 1 and 0, respectively. The simulation should be run for 10 half-lives, with output every half-life. Simulated concentrations should match those in Table 2 (to the model's numerical precision, usually 6 significant figures).

Table 2 - Unit concentration response

Time	Unit Concentration Response			
	Decay Reactions		Growth Reactions	
half-lives	Reactant mg/L	Product mg/L	Reactant mg/L	Product mg/L
0	1	0	1024	1
1	0.5	0.5	1023	2
2	0.25	0.75	1021	4
3	0.125	0.875	1017	8
4	0.0625	0.9375	1009	16
5	0.03125	0.96875	993	32
6	0.015625	0.984375	961	64
7	0.0078125	0.9921875	897	128
8	0.00390625	0.99609375	769	256
9	0.001953125	0.998046875	513	512
10	0.0009765625	0.999023438	1	1024

Test 2.1 – Phytoplankton Respiration

In a static system with phytoplankton respiration and no growth, death, excretion, or settling, initial concentrations of phytoplankton C, N and P, should decline at the specified first-order respiration rate. With all other carbon and nutrient cycling reactions set to 0, TIOC, NH_4, and PO_4 should accumulate at that same rate.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that all carbon and nutrient cycling reaction rate constants are set to 0. Set the respiration temperature correction factor to 1.08, and the input respiration rate constant and water temperature so that the reaction half life is 5 days. This test should be repeated for each of the following combinations of respiration rate constant and water temperature and for each of the phytoplankton groups:

- $k_R = 0.299291$ day^{-1}, T = 10 C
- $k_R = 0.138629$ day^{-1}, T = 20 C
- $k_R = 0.0642123$ day^{-1}, T = 30 C

Set the following initial concentrations. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- NH_4: 0 mg/L
- NO_3: 0 mg/L
- Detrital N: 0 mg/L
- Dissolved organic N: 0 mg/L
- PO_4: 0 mg/L
- Detrital P: 0 mg/L
- Dissolved organic P: 0 mg/L
- $CBOD_f$, $CBOD_s$: 0 mg/L
- TIOC: 0 mg/L
- Or, pH 7.7, alkalinity 100 mg/L: TIOC = 25.143, 24.891, 24.739 mg/L for T = 10, 20, 30 C

Run the simulation for duration 50 days (i.e., 10 half-lives). Check phytoplankton C, N, and P, ΔTIOC, NH_4, and PO_4 concentrations to match the analytical solutions in Table 3.

Table 3 - Unit concentration response

Time	Concentration					
days	Phyto C mg/L	Phyto N mg/L	Phyto P mg/L	ΔTIOC mg/L	NH_4 mg/L	PO_4 mg/L
0	1.000000	0.200000	0.050000	0.000000	0.000000	0.000000
5	0.500000	0.100000	0.025000	0.500000	0.100000	0.025000
10	0.250000	0.050000	0.012500	0.750000	0.150000	0.037500
15	0.125000	0.025000	0.006250	0.875000	0.175000	0.043750
20	0.062500	0.012500	0.003125	0.937500	0.187500	0.046875
25	0.031250	0.006250	0.001563	0.968750	0.193750	0.048438
30	0.015625	0.003125	0.000781	0.984375	0.196875	0.049219
50	0.000977	0.000195	0.000049	0.999023	0.199805	0.049951

Test 2.2a – Phytoplankton Death: WQCBM and WQADD OC Pathways

In a static system with phytoplankton death and no growth, respiration, excretion, or settling, initial concentrations of phytoplankton C should decline at the specified first-order death rate. With all other carbon cycling reactions set to 0, TOC should accumulate at that same rate. In WQCBM, TOC is distributed between two CBOD fractions and three POC fractions following user-specified ratios. In WQADD, TOC is distributed between labile POC and DOC fractions (LPOM, LDOM) following a user-specified ratio.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that all carbon cycling reaction rate constants are set to 0:

- CBOD_f and CBOD_s decay
- Denitrification
- OC_P_f and OC_P_s hydrolysis
- LDOM, PDOM transformation
- LDOM, PDOM decay

- LPOM dissolution

Set the death temperature correction factor to 1.08, and the input death rate constant and water temperature so that the reaction half-life is 10 days. In WQCBM, set the foc parameter to 0.4 so that 40% of the phytoplankton carbon is allocated to CBOD. Set the fd5 parameter to 0.5 so that the carbon allocated to CBOD is allocated equally between CBOD_f and CBOD_s. Set the fd9f, fd9s, and fd9r parameters to 0.333333 so that the carbon allocated to POC is distributed equally to OC_P_f, OC_P_s, and OC_P_r. In WQADD, set the Pam parameter to 0.6 so that the 60% of the carbon is allocated to PDOM and 40% to LDOM.

This test should be repeated for each of the following combinations of death rate constant and water temperature and for each of the phytoplankton groups:

- $k_D = 0.149645$ day^{-1}, T = 10 C
- $k_D = 0.0693147$ day^{-1}, T = 20 C
- $k_D = 0.0321061$ day^{-1}, T = 30 C

Set the following initial concentrations. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- OC_P_f, OC_P_s, OC_P_r: 0 mg/L
- CBOD_f, CBOD_s: 0 mg/L
- LPOM, LDOM: 0 mg/L

Run the simulation for duration 100 days (i.e., 10 half-lives). Check phytoplankton C, $CBOD_i$, POC_i, LPOM, and LDOM concentrations to match the analytical solutions in Table 4.

Table 4 - Unit concentration response

Time	Concentration				
days	Phyto C mg/L	$CBOD_i$ mg/L	OC_i mg/L	LPOM mg/L	LDOM mg/L
0	1.000000	0.000000	0.000000	0.000000	0.000000
10	0.500000	0.533333	0.100000	0.300000	0.200000
20	0.250000	0.800000	0.150000	0.450000	0.300000
30	0.125000	0.933333	0.175000	0.525000	0.350000
40	0.062500	1.000000	0.187500	0.562500	0.375000
50	0.031250	1.033333	0.193750	0.581250	0.387500
60	0.015625	1.050000	0.196875	0.590625	0.393750
100	0.000977	1.065625	0.199805	0.599414	0.399609

Test 2.2b – Phytoplankton Death: WQCBM Nutrient Pathways

In a static system with phytoplankton death and no growth, respiration, excretion, or settling, initial concentrations of phytoplankton N and P should decline at the specified first-order death rate. With all other nutrient cycling reactions set to 0, TON and TOP should accumulate at that same rate. In WQCBM, TON is distributed between ON_P and ON_D, and TOP is distributed between OP_P and OP_D following user-specified ratios.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that all nutrient cycling reaction rate constants are set to 0. Set the death temperature correction factor to 1.08, and the input death rate constant and water temperature so that the reaction half life is 10 days. Set the fon and fop parameters to 0.4, so that 40% of the phytoplankton nitrogen and phosphorus are allocated to ON_D and OP_D, respectively. This test should be repeated for each of the following combinations of death rate constant and water temperature and for each of the phytoplankton groups:

- $k_D = 0.149645\ day^{-1}$, T = 10 C
- $k_D = 0.0693147\ day^{-1}$, T = 20 C
- $k_D = 0.0321061\ day^{-1}$, T = 30 C

Set the following initial concentrations. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- ON_P: 0 mg/L
- ON_D: 0 mg/L
- OP_P: 0 mg/L
- OP_D: 0 mg/L

Run the simulation for duration 100 days (i.e., 10 half-lives). Check concentrations of phytoplankton N, phytoplankton P, ON_P, ON_D, OP_P, and OP_D to match the analytical solutions in Table 5.

Table 5 - Unit concentration response

Time	Concentration			
days	Phyto N mg/L	Phyto P mg/L	ON_P, ON_D mg/L	OP_P, OP_D mg/L
0	0.200000	0.050000	0.000000	0.000000
10	0.100000	0.025000	0.050000	0.012500
20	0.050000	0.012500	0.075000	0.018750
30	0.025000	0.006250	0.087500	0.021875
40	0.012500	0.003125	0.093750	0.023438
50	0.006250	0.001563	0.096875	0.024219
60	0.003125	0.000781	0.098438	0.024609
100	0.000195	0.000049	0.099902	0.024976

Test 2.3 – Phytoplankton Grazing: linear option

In a static system with phytoplankton grazing and no growth, respiration, excretion, death, or settling, initial concentrations of phytoplankton C, N, and P should decline at the specified first-order grazing rate. With all other carbon and nutrient cycling reactions set to 0, POC, PON, and POP should accumulate at that same rate. In WQCBM, separate rate constants for micro-grazing and macro-grazing can be specified. Grazed phytoplankton carbon is distributed between three POC fractions following user-specified ratios.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that all particulate carbon, nitrogen, and phosphorus cycling reaction rate constants are set to 0:

- OC_P_f and OC_P_s hydrolysis
- ON_P, OP_P hydrolysis

Set the grazing temperature correction factor to 1.08, and the input grazing rate constant and water temperature so that the reaction half-life is 10 days. Set the fg9f, fg9s, and fg9r parameters to 0.333333 so that the carbon is distributed equally to OC_P_f, OC_P_s, and OC_P_r.

This test should be repeated for each of the following combinations of grazing rate constant and water temperature, for micro-grazing and macro-grazing, and for each of the phytoplankton groups:

- $k_G = 0.149645$ day^{-1}, T = 10 C
- $k_G = 0.0693147$ day^{-1}, T = 20 C
- $k_G = 0.0321061$ day^{-1}, T = 30 C

Set the following initial concentrations. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- OC_P_f, OC_P_s, OC_P_r: 0 mg/L
- ON_P, OP_P: 0 mg/L

Run the simulation for duration 100 days (i.e., 10 half-lives). Check phytoplankton C, N, and P, and OC_P_i, ON_P, and OP_P concentrations to match the analytical solutions in Table 6.

Table 6 - Unit concentration response

Time	Concentration					
days	Phyto C mg/L	Phyto N mg/L	Phyto P mg/L	OC_P_i mg/L	ON_P mg/L	OP_P mg/L
0	1.000000	0.200000	0.050000	0.000000	0.000000	0.000000
10	0.500000	0.100000	0.025000	0.166667	0.100000	0.025000
20	0.250000	0.050000	0.012500	0.250000	0.150000	0.037500
30	0.125000	0.025000	0.006250	0.291667	0.175000	0.043750
40	0.062500	0.012500	0.003125	0.312500	0.187500	0.046875
50	0.031250	0.006250	0.001563	0.322917	0.193750	0.048438
60	0.015625	0.003125	0.000781	0.328125	0.196875	0.049219
100	0.000977	0.000195	0.000049	0.333008	0.199805	0.049951

Test 2.4a – Detrital Dissolution in WQCBM

In a static system with particulate detrital hydrolysis and no settling and no phytoplankton death, initial concentrations of POC, PON and POP should decline at the specified first-order hydrolysis rate. With all other organic carbon and nutrient cycling reactions set to 0, CBOD, DON and DOP should accumulate at that same rate. In WQCBM, OC_P_f and OC_P_s are hydrolyzed to CBOD_s, ON_P is hydrolyzed to ON_D, and OP_P is hydrolyzed to OP_D.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that all nutrient cycling reaction rate constants are set to 0. Set the hydrolysis temperature correction factors to 1.08, and the input hydrolysis rate constants and water temperature so that the reaction half lives are 5 days. This test should be repeated for each of the following combinations of hydrolysis rate constant and water temperature:

- $k_H = 0.299291\ day^{-1}$, T = 10 C
- $k_H = 0.138629\ day^{-1}$, T = 20 C
- $k_H = 0.0642123\ day^{-1}$, T = 30 C

Set the following initial concentrations:

- OC_P_f: 1 mg/L
- OC_P_s: 1 mg/L
- ON_P: 1 mg/L
- OP_P: 1 mg/L
- CBOD_s: 0 mg/L
- CBOD_f: 0 mg/L
- ON_D: 0 mg/L
- OP_D: 0 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of OC_P_f, OC_P_s, ON_P, OP_P, CBOD, ON_D, and OP_D to match the analytical solutions in Table 7.

Table 7 - Unit concentration response

Time	Concentration			
days	OC_P_i mg/L	ON_P, OP_P mg/L	CBOD mg/L	ON_D, OP_D mg/L
0	1.000000	1.000000	0.000000	0.000000
5	0.500000	0.500000	1.333333	0.500000
10	0.250000	0.250000	2.000000	0.750000
15	0.125000	0.125000	2.333333	0.875000
20	0.062500	0.062500	2.500000	0.937500
25	0.031250	0.031250	2.583333	0.968750
30	0.015625	0.015625	2.625000	0.984375
50	0.000977	0.000977	2.664062	0.999023

Test 2.4b – Detrital Dissolution in WQADD

In a static system with particulate organic matter dissolution and no settling or phytoplankton death, initial concentrations of POM should decline at the specified first-order dissolution rate. With all other organic matter reactions set to 0, DOM should accumulate at that same rate. In WQADD (version 2), LPOM and RPOM are dissolved with no transformation to LDOM and RDOM, respectively.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that LPOM and LDOM transformation rate constants and all OM decay rate constants are set to 0. Set the dissolution temperature correction factors to 1.08, and the input dissolution rate constants and water temperature so that the reaction half lives are 5 days. This test should be repeated for each of the following combinations of dissolution rate constant and water temperature:

- k_{diss} = 0.299291 day^{-1}, T = 10 C
- k_{diss} = 0.138629 day^{-1}, T = 20 C
- k_{diss} = 0.0642123 day^{-1}, T = 30 C

Set the following initial concentrations:

- LPOM: 1 mg/L
- RPOM: 1 mg/L
- LDOM: 0 mg/L
- RDOM: 0 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of LPOM, RPOM, LDOM, and RDOM to match the analytical solutions in Table 8. Note that LDOM and RDOM will remain at 0 if the dissolution reaction is not updated from decay to transformation.

Table 8 - Unit concentration response

Time	Concentration			
days	LPOM mg/L	RPOM mg/L	LDOM mg/L	RDOM mg/L
0	1.000000	1.000000	0.000000	0.000000
5	0.500000	0.500000	0.500000	0.500000
10	0.250000	0.250000	0.750000	0.750000
15	0.125000	0.125000	0.875000	0.875000
20	0.062500	0.062500	0.937500	0.937500
25	0.031250	0.031250	0.968750	0.968750
30	0.015625	0.015625	0.984375	0.984375
50	0.000977	0.000977	0.999023	0.999023

Test 2.4c – POM Transformation in WQADD

In a static system with labile organic matter transformation and no settling or phytoplankton death, initial concentrations of labile POM and DOM should decline at the specified first-order transformation rate. With all other organic matter reactions set to 0, refractory POM and DOM should accumulate at that same rate. In WQADD, LPOM and LDOM are transformed to RPOM and RDOM, respectively.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that LPOM and RPOM dissolution rate constants and all OM decay rate constants are set to 0. Set the transformation temperature correction factors to 1.08, and the input transformation rate constants and water temperature so that the reaction half lives are 5 days. This test should be repeated for each of the following combinations of transformation rate constant and water temperature:

- k_{trans} = 0.299291 day^{-1}, T = 10 C
- k_{trans} = 0.138629 day^{-1}, T = 20 C
- k_{trans} = 0.0642123 day^{-1}, T = 30 C

Set the following initial concentrations:

- LPOM: 1 mg/L
- LDOM: 1 mg/L
- RPOM: 0 mg/L
- RDOM: 0 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of LPOM, LDOM, RPOM, and RDOM to match the analytical solutions in Table 9.

Table 9 - Unit concentration response

Time	Concentration			
days	LPOM mg/L	LDOM mg/L	RPOM mg/L	RDOM mg/L
0	1.000000	1.000000	0.000000	0.000000
5	0.500000	0.500000	0.500000	0.500000
10	0.250000	0.250000	0.750000	0.750000
15	0.125000	0.125000	0.875000	0.875000
20	0.062500	0.062500	0.937500	0.937500
25	0.031250	0.031250	0.968750	0.968750
30	0.015625	0.015625	0.984375	0.984375
50	0.000977	0.000977	0.999023	0.999023

Test 2.5a – OM Mineralization and Decay in WQCBM

In a static system with dissolved organic matter decay and no phytoplankton or detritus reactions, the initial concentrations of CBOD, DON, and DOP should decline at the specified first-order mineralization and decay rates. With all other inorganic carbon and nutrient cycling reactions set to 0, TIOC, NH_4, and PO_4 should accumulate at those same rates. In WQCBM, CBOD_f and CBOD_s decay to TIOC, ON_D mineralizes to NH3, and OP_D mineralizes to PO4.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton growth, respiration, excretion, death, and grazing rate constants are set to 0. Specify temperature correction factors of 1.08 for CBOD_f decay, CBOD_s decay, ON_D mineralization and OP_D mineralization. Specify water temperature and rate constants so that reaction half lives are 5 days for CBOD_f decay, CBOD_s decay, ON_D mineralization and OP_D mineralization. Set all other WQCBM carbon and nutrient cycling reaction rate constants, including reaeration to 0. To ensure that oxygen levels will not affect the CBOD oxidation rates, set the DO half-saturation coefficient for deoxygenation, *kbod*, to 0. Make sure that decay rates for LPOM, RPOM, LDOM, and RDOM in WQADD are 0. This test should be repeated for each of the following combinations of decay/mineralization rate constant and water temperature:

- k_{decay} = 0.299291 day^{-1}, T = 10 C
- k_{decay} = 0.138629 day^{-1}, T = 20 C
- k_{decay} = 0.0642123 day^{-1}, T = 30 C

Set the following initial concentrations:

- DO: 10 mg/L
- CBOD_f: 1.333333 mg/L
- CBOD_s: 1.333333 mg/L
- ON_D: 1 mg/L
- OP_D: 1 mg/L
- TIOC: 0 mg/L
- NH_4: 0 mg/L

- PO_4: 0 mg/L
- TIOC: 0 mg/L
- Or, pH 7.7, alkalinity 100 mg/L: TIOC = 25.143, 24.891, 24.739 mg/L for T = 10, 20, 30 C

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of CBOD (total), ON_D, OP_D, ΔTIOC, NH_4, and PO_4 to match the analytical solutions in Table 10.

Table 10 - Unit concentration response

Time	Concentration			
days	CBOD(total) mg/L	ON_D, OP_D mg/L	ΔTIOC mg/L	NH_4, PO_4 mg/L
0	2.666667	1.000000	0.000000	0.000000
5	1.333333	0.500000	0.500000	0.500000
10	0.666667	0.250000	0.750000	0.750000
15	0.333333	0.125000	0.875000	0.875000
20	0.166667	0.062500	0.937500	0.937500
25	0.083333	0.031250	0.968750	0.968750
30	0.041667	0.015625	0.984375	0.984375
50	0.002604	0.000977	0.999023	0.999023

Test 2.5b – Detrital Dissolution in WQADD

In a static system with organic matter decay and no phytoplankton or other organic matter reactions, the initial concentrations of OM (labile and refractory, particulate and dissolved) should decline at the specified first-order decay rates. With all other inorganic carbon reactions set to 0, TIOC should accumulate at those same rates. In WQADD, LPOM, RPOM, LDOM, and RDOM all decay to TIOC.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that all phytoplankton rate constants are set to 0. Specify temperature correction factors of 1.08 for LPOM decay, RPOM decay, LDOM decay, and RDOM decay. Specify water temperature and rate constants so that reaction half lives are 5 days for LPOM decay, RPOM decay, LDOM decay, and RDOM decay. Set all other WQADD carbon cycling reaction rate constants to 0, including LPOM and LDOM transformation, LPOM and RPOM dissolution, and reaeration. Make sure that decay rates for CBOD_f and CBOD_s in WQCBM are 0. This test should be repeated for each of the following combinations of decay rate constant and water temperature:

- k_{decay} = 0.299291 day^{-1}, T = 10 C
- k_{decay} = 0.138629 day^{-1}, T = 20 C
- k_{decay} = 0.0642123 day^{-1}, T = 30 C

Set the following initial concentrations:

- LPOM: 1 mg/L
- RPOM: 1 mg/L
- LDOM: 1 mg/L
- RDOM: 1 mg/L
- TIOC: 0 mg/L
- Or, pH 7.7, alkalinity 100 mg/L: TIOC = 25.143, 24.891, 24.739 mg/L for T = 10, 20, 30 C

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of LPOM, RPOM, LDOM, RDOM, and ΔTIOC to match the analytical solutions in Table 11.

Table 11 - Unit concentration response

Time	Concentration	
days	OM classes mg/L	ΔTIOC mg/L
0	1.000000	0.000000
5	0.500000	2.000000
10	0.250000	3.000000
15	0.125000	3.500000
20	0.062500	3.750000
25	0.031250	3.875000
30	0.015625	3.937500
50	0.000977	3.996094

Test 2.6a – Inorganic N Reactions: Nitrification

In a static system with nitrification and no phytoplankton or organic nitrogen reactions, the initial concentration of NH_4 should decline at the specified first-order nitrification rate. With denitrification set to 0, NO_3 should accumulate at that same rate. Nitrification consumes oxygen, and lower DO levels inhibit the nitrification reaction.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton growth, respiration, and excretion rate constants are set to 0. Specify a nitrification temperature correction factor of 1.08, and specify water temperature and nitrification rate constants so that reaction half lives are 5 days. Set all other WQCBM nutrient cycling reaction rate constants to 0. Make sure that the simulation of dissolved oxygen is bypassed in this test. Set the oxygen half-saturation constant *knit* to 2 and the DO concentration to 2 so that input nitrification rates are reduced by half. This test should be repeated for each of the following combinations of nitrification rate constant and water temperature:

- k_{nitr} = 0.598582 day^{-1}, T = 10 C
- k_{nitr} = 0.277258 day^{-1}, T = 20 C
- k_{nitr} = 0.128425 day^{-1}, T = 30 C

Set the following initial concentrations:

- DO: 2 mg/L
- NH_4: 1 mg/L
- NO_3: 0 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of NH_4 and NO_3 to match the analytical solutions in Table 12.

Table 12 - Unit concentration response

Time	Concentration	
days	NH_4 mg/L	NO_3 mg/L
0	1.000000	0.000000
5	0.500000	0.500000
10	0.250000	0.750000
15	0.125000	0.875000
20	0.062500	0.937500
25	0.031250	0.968750
30	0.015625	0.984375
50	0.000977	0.999023

Test 2.6b – Inorganic N Reactions: Denitrification

In a static system with denitrification and no phytoplankton or nitrification reactions, the initial concentration of NO_3 should decline at the specified first-order denitrification rate. Denitrification consumes CBOD, and higher DO levels inhibit the nitrification reaction.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton growth rate constant is set to 0. Specify a denitrification temperature correction factor of 1.08, and specify water temperature and denitrification rate constants so that reaction half lives are 5 days. Set all other WQCBM nutrient cycling reaction rate constants to 0. Make sure that the simulation of dissolved oxygen is bypassed in this test. Set the oxygen half-saturation constant *kno3* to 2 and the DO concentration to 2 so that input denitrification rates are reduced by half. This test should be repeated for each of the following combinations of denitrification rate constant and water temperature:

- $k_{nitr} = 0.598582\ day^{-1}$, T = 10 C
- $k_{nitr} = 0.277258\ day^{-1}$, T = 20 C
- $k_{nitr} = 0.128425\ day^{-1}$, T = 30 C

Set the following initial concentrations:

- DO: 2 mg/L
- NO_3: 1 mg/L
- CBOD: 2.857143 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of NO_3 and CBOD_f to match the analytical solutions in Table 13.

Table 13 - Unit concentration response

Time	Concentration	
days	NO_3 mg/L	CBOD_f mg/L
0	1.000000	2.857143
5	0.500000	1.428571
10	0.250000	0.714286
15	0.125000	0.357143
20	0.062500	0.178571
25	0.031250	0.089286
30	0.015625	0.044643
50	0.000977	0.002790

Test 2.7a – Phytoplankton Growth, no limitation

In a static system with phytoplankton growth and no respiration, excretion, death, or settling, initial concentrations of phytoplankton C should increase at the specified first-order growth rate until nutrients or light become limiting. Initial concentrations of DIN and DIP should decline at the same rate.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton respiration, death, excretion, and grazing rate constants are set to 0. Specify a growth temperature correction factor of 1.08, and specify water temperature and growth rate constants so that reaction doubling times are 1 day. To assure no significant light or nutrient limitation, select the Steele light limitation formula and specify the following coefficients:

- Light saturation constant: 100 W/m^2 (or 200 Ly/day)
- Light extinction coefficient: 0.000001 m^{-1}
- Half-saturation constant for N limitation: 0.000001 mg/L
- Half-saturation constant for P limitation: 0.0000002 mg/L
- D:C ratio: 2
- N:C ratio: 0.2
- P:C ratio: 0.05
- Chl:C ratio: 0.02 (i.e., C:Chl = 50)

Make sure that total incoming light at the surface after reflectance loss is constant and equal to twice the light saturation constant:

- Incident light: 200 W/m^2 (or 400 Ly/day)
- Fraction PAR: 50%
- Albedo: 0
- Fraction daylight: 1.0

This test should be repeated for each of the following combinations of growth rate constant and water temperature:

- k_G = 1.496453 day^{-1}, T = 10 C
- k_G = 0.693147 day^{-1}, T = 20 C
- k_G = 0.321061 day^{-1}, T = 30 C

Set the following initial concentrations:

- Phytoplankton C: 0.0001 mg/L
- Phytoplankton N: 0.000002 mg/L
- Phytoplankton P: 0.0000005 mg/L
- NH_4: 1.002048 mg/L
- NO_3: 0 mg/L
- PO_4: 1.000512 mg/L

Run the simulation for duration 10 days (i.e., 10 half-lives). Check phytoplankton C, N, and P, and NH4, NO3, and PO4 concentrations to match the analytical solutions in Table 14.

Table 14 - Unit concentration response

Time	Concentration					
days	Phyto C mg/L	Phyto N mg/L	Phyto P mg/L	NH3 mg/L	NO3 mg/L	PO4 mg/L
0	0.0001	0.00002	0.000005	1.002048	0	1.0005120
1	0.0002	0.00004	0.00001	1.002046	0	1.0005115
2	0.0004	0.00008	0.00002	1.002042	0	1.0005105
3	0.0008	0.00016	0.00004	1.002034	0	1.0005085
4	0.0016	0.00032	0.00008	1.002018	0	1.0005045
5	0.0032	0.00064	0.00016	1.001986	0	1.0004965
6	0.0064	0.00128	0.00032	1.001922	0	1.0004805
7	0.0128	0.00256	0.00064	1.001794	0	1.0004485
8	0.0256	0.00512	0.00128	1.001538	0	1.0003845
9	0.0512	0.01024	0.00256	1.001026	0	1.0002565
10	0.1024	0.02048	0.00512	1.000002	0	1.0000005

Run the simulation again switching the initial concentrations of NH3 and NO3. The NO3 response should follow the NH3 column in Table 14.

In GenAlgae, algal growth follows the "Topt" temperature correction function:

$$k_{G,T} = k_{G,Topt} \cdot e^{-\kappa 1 (T - Topt)^2} \qquad for\ T < Topt$$

$$k_{G,T} = k_{G,Topt} \cdot e^{-\kappa 2 (Topt - T)^2} \qquad for\ T > Topt$$

For testing purposes, a value for $\kappa 1$ can be derived to duplicate the "theta" temperature correction function:

$$e^{-\kappa 1 (T-Topt)^2} = \theta^{T-20}$$

$$\kappa 1 = -\ln\theta \frac{T-20}{(T-Topt)^2}$$

For *Topt* of 20C and θ of 1.08, the equivalent value for $\kappa 1$ is 0.0076961. If $\kappa 2$ is set to this same value, the temperature correction for 30C will be the same as for 10C. To test GenAlgae growth, specify these temperature correction coefficients, and then repeat the tests for each of the following combinations of growth rate constant and water temperature:

- k_G = 1.496453 day^{-1}, T = 10 C
- k_G = 0.693147 day^{-1}, T = 20 C
- k_G = 1.496453 day^{-1}, T = 30 C

Results should match the analytical solutions in Table 14.

Test 2.7b – Phytoplankton Growth, light limitation

In a static system with phytoplankton growth and no respiration, excretion, death, or settling, and with average water column light intensity greater or less than the phytoplankton light coefficient, initial concentrations of phytoplankton C should increase at a fraction of the specified first-order growth rate until nutrients or light become limiting. Initial concentrations of DIN and DIP should decline at the same rate. Three light limitation options are provided in WQCBM. The equations are taken from the QUAL2K Documentation (Chapra, et al., 2009):

1. Half-Saturation Equation

$$\phi_{Lp} = \frac{1}{k_e H}\ln\left(\frac{K_{Lp} + I(0)}{K_{Lp} + I(0)e^{-k_e H}}\right)$$

2. Smith Equation

$$\phi_{Lp} = \frac{1}{k_e H}\ln\left(\frac{I(0)/K_{Lp} + \sqrt{1+\left(I(0)/K_{Lp}\right)^2}}{\left(I(0)/K_{Lp}\right)e^{-k_e H} + \sqrt{1+\left(\left(I(0)/K_{Lp}\right)e^{-k_e H}\right)^2}}\right)$$

3. Steele Equation

$$\phi_{Lp} = \frac{e}{k_e H}\left(e^{-\frac{I(0)}{K_{Lp}}e^{-k_e H}} - e^{-\frac{I(0)}{K_{Lp}}}\right)$$

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton respiration, death, excretion, and grazing

rate constants are set to 0. Specify a growth temperature correction factor of 1.0, and specify incident light intensity and growth rate constants so that reaction doubling times are 1 day. To assure no significant nutrient limitation, specify the following coefficients:

- Half-saturation constant for N limitation: 0.000001 mg/L
- Half-saturation constant for P limitation: 0.0000002 mg/L
- D:C ratio: 2
- N:C ratio: 0.2
- P:C ratio: 0.05
- Chl:C ratio: 0.02 (i.e., C:Chl = 50)

Set the following light parameters, making sure that total incoming light at the surface after reflectance loss is constant:

- Incident light intensity: 100, 200, 400 W/m^2
- Half-saturation and Smith light constant: 50 W/m^2
- Steele light saturation constant: 100 W/m^2
- Light extinction coefficient: 0.000001 m^{-1}
- Fraction PAR: 50%
- Albedo: 0
- Fraction daylight: 1.0

For the range of light intensity and the parameters, the three light limitation equations give the following growth rate reductions:

Table 15 – Light limitation factors for selected parameters and incident light

Total Light	PAR Light	Light Limitation Factors		
W/m^2	W/m^2	Half-Saturation	Smith	Steele
100	50	0.500000	0.707107	0.824360
200	100	0.666667	0.894427	1.000000
400	200	0.800000	0.970142	0.735759

This test should be repeated for each of the light limitation equations. For the Half-Saturation equation, test for the following combinations of growth rate constant and total incident light:

- $k_G = 1.386294\ day^{-1}$, $I_0 = 100\ W/m^2$
- $k_G = 1.039721\ day^{-1}$, $I_0 = 200\ W/m^2$
- $k_G = 0.866434\ day^{-1}$, $I_0 = 400\ W/m^2$

For the Smith equation, test for the following combinations of growth rate constant and total incident light:

- $k_G = 0.980258\ day^{-1}$, $I_0 = 100\ W/m^2$
- $k_G = 0.774962\ day^{-1}$, $I_0 = 200\ W/m^2$
- $k_G = 0.714480\ day^{-1}$, $I_0 = 400\ W/m^2$

For the Steele equation, test for the following combinations of growth rate constant and total incident light:

- $k_G = 0.840831\ day^{-1}$, $I_0 = 100\ W/m^2$

- $k_G = 0.693147$ day^{-1}, $I_0 = 200$ W/m^2
- $k_G = 0.942085$ day^{-1}, $I_0 = 400$ W/m^2

Set the following initial concentrations:

- Phytoplankton C: 0.0001 mg/L
- Phytoplankton N: 0.000002 mg/L
- Phytoplankton P: 0.0000005 mg/L
- NH_4: 1.002048 mg/L
- NO_3: 0 mg/L
- PO_4: 1.000512 mg/L

Run the simulation for duration 10 days (i.e., 10 half-lives). Check phytoplankton C, N, and P, and NH4, NO3, and PO4 concentrations to match the analytical solutions in Table 16.

Table 16 - Unit concentration response

Time	Concentration					
days	Phyto C mg/L	Phyto N mg/L	Phyto P mg/L	NH3 mg/L	NO3 mg/L	PO4 mg/L
0	0.0001	0.00002	0.000005	1.002048	0	1.0005120
1	0.0002	0.00004	0.00001	1.002046	0	1.0005115
2	0.0004	0.00008	0.00002	1.002042	0	1.0005105
3	0.0008	0.00016	0.00004	1.002034	0	1.0005085
4	0.0016	0.00032	0.00008	1.002018	0	1.0005045
5	0.0032	0.00064	0.00016	1.001986	0	1.0004965
6	0.0064	0.00128	0.00032	1.001922	0	1.0004805
7	0.0128	0.00256	0.00064	1.001794	0	1.0004485
8	0.0256	0.00512	0.00128	1.001538	0	1.0003845
9	0.0512	0.01024	0.00256	1.001026	0	1.0002565
10	0.1024	0.02048	0.00512	1.000002	0	1.0000005

Test 2.7c – Phytoplankton Growth, light extinction

In a static system with net phytoplankton growth and excess nutrients, phytoplankton concentrations rise until self-shading increases light extinction and reduces light intensity enough to become limiting. When the light-limited growth rate is balanced by equal respiration rate in the absence of excretion, death, or settling, concentrations of phytoplankton C, N, P, chlorophyll, and light extinction coefficient should remain constant. In WQCBM, light extinction coefficient K_e in m^{-1} given by:

$$K_e = K_{eb} + a_{shd}\, Chl^{bshd}$$

where K_{eb} is background light extinction coefficient, m^{-1}, a_{shd} is the self-shading multiplier, and b_{shd} is the self-shading exponent.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton death, excretion, and grazing rate constants are set to 0. Specify growth and respiration temperature correction factors of 1.0, and set respiration rate constant to 0.346574 for a half-life of 2 days. Specify light parameters and growth rate constants so that reaction doubling times are 2 days. To assure no significant nutrient limitation, specify the following coefficients:

- Half-saturation constant for N limitation: 0.000001 mg/L
- Half-saturation constant for P limitation: 0.0000002 mg/L
- D:C ratio: 2
- N:C ratio: 0.2
- P:C ratio: 0.05
- Chl:C ratio: 0.02 (i.e., C:Chl = 50)

Set the following light parameters, making sure that total incoming light at the surface after reflectance loss is constant:

- Incident light intensity: 200 W/m^2
- Half-saturation and Smith light constant: 50 W/m^2
- Steele light saturation constant: 100 W/m^2
- Background light extinction coefficient: 0.5 m^{-1}
- Self-shading multiplier: 0.06
- Self-shading exponent: 0.7
- Fraction PAR: 50%
- Fraction daylight: 1.0

For the range of phytoplankton concentration and the specified parameters, the three light limitation equations give the following growth rate reductions:

Table 17 – Light limitation factors for selected parameters and incident light

Phyto C	Phyto Chl	Light Extinction	Light Limitation Factors		
mg/L	µg/L	m^{-1}	Half-Saturation	Smith	Steele
0.5	10	0.800712	0.571744	0.794596	0.917897
2.5	50	1.427748	0.495028	0.686855	0.797480
5.0	100	2.007132	0.428762	0.586918	0.685802

This test should be repeated for each of the light limitation equations. For the Half-Saturation equation, test for the following combinations of growth rate constant and phytoplankton concentration:

- k_G = 0.606170 day^{-1}, Phyto = 0.5 mgC/L
- k_G = 0.700109 day^{-1}, Phyto = 2.5 mgC/L
- k_G = 0.808312 day^{-1}, Phyto = 5.0 mgC/L

For the Smith equation, test for the following combinations of growth rate constant and total incident light:

- k_G = 0.436164 day^{-1}, Phyto = 0.5 mgC/L

- k_G = 0.504580 day^{-1}, Phyto = 2.5 mgC/L
- k_G = 0.590497 day^{-1}, Phyto = 5.0 mgC/L

For the Steele equation, test for the following combinations of growth rate constant and total incident light:

- k_G = 0.377573 day^{-1}, Phyto = 0.5 mgC/L
- k_G = 0.434586 day^{-1}, Phyto = 2.5 mgC/L
- k_G = 0.505355 day^{-1}, Phyto = 5.0 mgC/L

In the three test simulations, set the following initial concentrations:

- Phytoplankton C: 0.5, 2.5, 5.0 mg/L
- Phytoplankton N: 0.1, 0.5, 1.0 mg/L
- Phytoplankton P: 0.025, 0.125, 0.25 mg/L
- NH_4: 1.0 mg/L
- NO_3: 0 mg/L
- PO_4: 1.0 mg/L

Run the simulation for duration 10 days (i.e., 10 half-lives). Check for constant phytoplankton C, N, and P, and NH4, NO3, and PO4 concentrations.

Test 2.7d – Phytoplankton Growth, nutrient limitation

In a static system with phytoplankton growth and no respiration, excretion, death, or settling, initial concentrations of phytoplankton C should increase at the specified first-order growth rate until nutrients or light become limiting. Initial concentrations of DIN and DIP should decline at the same rate. If an essential nutrient concentration is equal to the half-saturation coefficient, the growth rate will be reduced by half.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that phytoplankton respiration, death, excretion, and grazing rate constants are set to 0. Specify a growth temperature correction factor of 1.0, and specify nutrient concentrations and growth rate constant so that reaction doubling times are 2 days. This is accomplished by setting the growth rate constant for a half life of 1 day, setting one nutrient concentration equal to its half-saturation coefficient, and bypassing simulation of that nutrient. To assure no significant light limitation, select the Steele light limitation formula and specify the following coefficients:

- Incident light: 200 W/m^2 (or 400 Ly/day)
- Light saturation constant: 100 W/m^2 (or 200 Ly/day)
- Light extinction coefficient: 0.000001 m^{-1}
- Fraction PAR: 50%
- Albedo: 0
- Fraction daylight: 1.0

Set the growth rate constant to 0.693147 day^{-1}, and specify the following nutrient coefficients:

- Half-saturation constant for N limitation: 0.01 mg/L
- Half-saturation constant for P limitation: 0.002 mg/L
- D:C ratio: 2
- N:C ratio: 0.2
- P:C ratio: 0.05
- Chl:C ratio: 0.02 (i.e., C:Chl = 50)

Set the following initial concentrations:

- Phytoplankton C: 0.0001 mg/L
- Phytoplankton N: 0.000002 mg/L
- Phytoplankton P: 0.0000005 mg/L

This test should be repeated for each of the following combinations of initial nutrient concentrations, bypassing simulation of the variable in bold:

- **PO_4 = 0.002 mg/L**, NH_4 = 1.002048 mg/L, NO_3 = 0 mg/L
- PO_4 = 1.000512, **NH_4 = 0.01 mg/L**, NO_3 = 0 mg/L
- PO_4 = 1.000512, NH_4 = 0 mg/L, **NO_3 = 0.01 mg/L**

Run the simulation for duration 20 days (i.e., 10 half-lives). Check phytoplankton C, N, and P, and NH4, NO3, and PO4 concentrations to match the analytical solutions in Table 18 (except for the bypassed nutrient, which should maintain a constant initial concentration).

Table 18 - Unit concentration response

Time	Concentration					
days	Phyto C mg/L	Phyto N mg/L	Phyto P mg/L	NH3 mg/L	NO3 mg/L	PO4 mg/L
0	0.0001	0.00002	0.000005	1.002048	0	1.0005120
2	0.0002	0.00004	0.00001	1.002046	0	1.0005115
4	0.0004	0.00008	0.00002	1.002042	0	1.0005105
6	0.0008	0.00016	0.00004	1.002034	0	1.0005085
8	0.0016	0.00032	0.00008	1.002018	0	1.0005045
10	0.0032	0.00064	0.00016	1.001986	0	1.0004965
12	0.0064	0.00128	0.00032	1.001922	0	1.0004805
14	0.0128	0.00256	0.00064	1.001794	0	1.0004485
16	0.0256	0.00512	0.00128	1.001538	0	1.0003845
18	0.0512	0.01024	0.00256	1.001026	0	1.0002565
20	0.1024	0.02048	0.00512	1.000002	0	1.0000005

Run the simulation again switching the initial concentrations of NH3 and NO3. The NO3 response should follow the NH3 column in Table 18.

Test 2.8a – Oxygen Depletion with CBOD decay

In a static system with CBOD decay, initial concentrations of CBOD should decline at the deoxygenation rate. With no reaeration, nitrification, sediment oxygen demand, and no phytoplankton growth, respiration, or excretion, the initial concentration of DO should decrease proportionally to the CBOD depletion. WQCBM includes separate variables for CBOD_f and CBOD_s, which decay at fast and slow rates, respectively.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that reaeration, nitrification, sediment oxygen demand, phytoplankton growth, respiration, excretion, death, and grazing rate constants are set to 0. Specify temperature correction factors of 1.0 for CBOD_f decay and CBOD_s decay. Specify CBOD_f decay rate constant to 0.138629 for a reaction half life of 5 days, and CBOD_s decay rate constant to 0.0693147 for a half life of 10 days. Set all other WQCBM carbon and nutrient cycling reaction rate constants, including reaeration to 0. To ensure that oxygen levels will not affect the CBOD oxidation rates, set the DO half-saturation coefficient for deoxygenation, *kbod*, to 0.

Set the following initial concentrations:

- DO: 10 mg/L
- CBOD_f: 5 mg/L
- CBOD_s: 1 mg/L

Run the simulation for duration 50 days. Check concentrations of CBOD_f, CBOD_s, and DO to match the analytical solutions in Table 19.

Table 19 - Unit concentration response

Time	Concentration		
days	CBOD_f mg/L	CBOD_s mg/L	DO mg/L
0	5.000000	1.000000	10.000000
5	2.500000	0.707107	7.207107
10	1.250000	0.500000	5.750000
15	0.625000	0.353553	4.978553
20	0.312500	0.250000	4.562500
25	0.156250	0.176777	4.333027
30	0.078125	0.125000	4.203125
50	0.004883	0.031250	4.036133

Test 2.8b – Oxygen Depletion with Nitrification

In a static system with nitrification, initial concentrations of NH_4 should decline at the nitrification rate. With no reaeration, CBOD decay, sediment oxygen demand, and no phytoplankton growth, respiration, or excretion, the initial concentration of DO should decrease at a ratio of 64/14 times the NH_4 depletion.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that reaeration, CBOD decay, sediment oxygen demand, phytoplankton growth, respiration, excretion, death, and grazing rate constants are set to 0. Specify temperature correction factors of 1.08 for nitrification. Specify water temperature and nitrification rate constants so that reaction half lives are 5 days. Set all other WQCBM nutrient cycling reaction rate constants, including reaeration to 0. To ensure that oxygen levels will not affect the nitrification rates, set the DO half-saturation coefficient for d nitrification, *knit*, to 0. This test should be repeated for each of the following combinations of nitrification rate constant and water temperature:

- k_{nitr} = 0.299291 day^{-1}, T = 10 C
- k_{nitr} = 0.138629 day^{-1}, T = 20 C
- k_{nitr} = 0.0642123 day^{-1}, T = 30 C

Set the following initial concentrations:

- DO: 10 mg/L
- NH3: 1.0 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of NH3 and DO to match the analytical solutions in Table 20.

Table 20 - Unit concentration response

Time	Concentration	
days	NH3 mg/L	DO mg/L
0	1.000000	10.000000
5	0.500000	7.714286
10	0.250000	6.571429
15	0.125000	6.000000
20	0.062500	5.714286
25	0.031250	5.571429
30	0.015625	5.500000
50	0.000977	5.433036

Test 2.8c – Oxygen Depletion with Phytoplankton Respiration

In a static system with phytoplankton respiration and no growth, death, excretion, settling, initial concentrations of phytoplankton C should decline at the specified first-order respiration rate. With no reaeration, CBOD decay, nitrification, and sediment oxygen demand, the initial concentration of DO should decrease at a ratio of 32/12 times the phytoplankton C depletion.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that reaeration, CBOD decay, nitrification, sediment oxygen demand, phytoplankton growth, excretion, death, and grazing rate constants are set to 0. Specify temperature correction factors of 1.08 for respiration. Specify water temperature

and respiration rate constants so that reaction half lives are 5 days. Set all other WQCBM nutrient cycling reaction rate constants, including reaeration to 0. This test should be repeated for each of the following combinations of respiration rate constant and water temperature and for each of the phytoplankton groups:

- k_R = 0.299291 day^{-1}, T = 10 C
- k_R = 0.138629 day^{-1}, T = 20 C
- k_R = 0.0642123 day^{-1}, T = 30 C

Set the following initial concentrations. Initial concentrations for phytoplankton can be assigned to any available group (e.g., diatoms, dinoflagellates) or divided among groups.

- Phytoplankton C: 1.0 mg/L
- Phytoplankton N: 0.2 mg/L
- Phytoplankton P: 0.05 mg/L
- DO: 10 mg/L

Run the simulation for duration 50 days (i.e., 10 half-lives). Check concentrations of Phytoplankton C and DO to match the analytical solutions in Table 21.

Table 21 - Unit concentration response

Time	Concentration	
days	Phyto C mg/L	DO mg/L
0	1.000000	10.000000
5	0.500000	8.666667
10	0.250000	8.000000
15	0.125000	7.666667
20	0.062500	7.500000
25	0.031250	7.416667
30	0.015625	7.375000
50	0.000977	7.335938

Test 2.8d – Oxygen Production with Phytoplankton Growth

In a static system with phytoplankton growth and no respiration, death, excretion, or settling, initial concentrations of phytoplankton C should increase at the specified first-order growth rate. With no reaeration, CBOD decay, nitrification, and sediment oxygen demand, the initial concentration of DO should increase at a ratio of *32/12* times the phytoplankton C growth when using NH_4. For growth using NO3, DO should increase at a ratio of *32(1/12 + 1.5 anc/14)* times the phytoplankton C growth, where *anc* is the phytoplankton nitrogen to carbon ratio.

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that reaeration, CBOD decay, nitrification, sediment oxygen demand, phytoplankton respiration, excretion, death, and grazing rate constants are set to 0. Specify temperature correction factors of 1.08 for growth. Specify water temperature

and growth rate constants so that reaction doubling times are 1 day. To assure no significant light or nutrient limitation, select the Steele light limitation formula and specify the following coefficients:

- Light saturation constant: 100 W/m^2 (or 200 Ly/day)
- Light extinction coefficient: 0.000001 m^{-1}
- Half-saturation constant for N limitation: 0.000001 mg/L
- Half-saturation constant for P limitation: 0.0000002 mg/L
- D:C ratio: 2
- N:C ratio: 0.2
- P:C ratio: 0.05
- Chl:C ratio: 0.02 (i.e., C:Chl = 50)

Make sure that total incoming light at the surface after reflectance loss is constant and equal to twice the light saturation constant:

- Incident light: 200 W/m^2 (or 400 Ly/day)
- Fraction PAR: 50%
- Albedo: 0
- Fraction daylight: 1.0

This test should be repeated for each of the following combinations of growth rate constant and water temperature:

- $k_G = 1.496453\ day^{-1}$, T = 10 C
- $k_G = 0.693147\ day^{-1}$, T = 20 C
- $k_G = 0.321061\ day^{-1}$, T = 30 C

Set the following initial concentrations:

- Phytoplankton C: 0.001 mg/L
- Phytoplankton N: 0.0002 mg/L
- Phytoplankton P: 0.00005 mg/L
- NH_4: 1.02048 mg/L, 0 mg/L
- NO_3: 0 mg/L, 1.02048 mg/L
- PO_4: 1.00512 mg/L
- DO: 5 mg/L

Run the simulation for duration 10 days (i.e., 10 half-lives) using NH_4 and then using NO_3. Check phytoplankton C and DO concentrations to match the analytical solutions in Table 22.

Table 22 - Unit concentration response

Time	Concentration		
days	Phyto C mg/L	DO with NH3 mg/L	DO with NO3 mg/L
0	0.0010	5.000000	5.000000
1	0.0020	5.002667	5.003352
2	0.0040	5.008000	5.010057
3	0.0080	5.018667	5.023467
4	0.0160	5.040000	5.050286
5	0.0320	5.082667	5.103924
6	0.0640	5.168000	5.211200
7	0.1280	5.338667	5.425752
8	0.2560	5.680000	5.854857
9	0.5120	6.362667	6.713067
10	1.0240	7.728000	8.429486

Test 2.8e – Oxygen Replenishment with Reaeration

In a static system with no phytoplankton or water quality reactions, initial dissolved oxygen deficit should decline at the calculated first-order reaeration rate, and dissolved oxygen concentration should approach saturation. Dissolved oxygen saturation is calculated as a function of salinity (PSU) and water temperature (K):

$$\ln C_{sat}(T,S) = -139.34411 + \frac{1.575701\times10^{5}}{T_a} - \frac{6.642308\times10^{7}}{T_a^2}$$

$$+ \frac{1.243800\times10^{10}}{T_a^3} - \frac{8.621949\times10^{11}}{T_a^4}$$

$$- \frac{S}{1.80655}\cdot\left(0.031929 - \frac{19.428}{T_a} + \frac{3.8673\times10^{2}}{T_a^2}\right)$$

Dissolved oxygen reaeration velocity (m/sec) is calculated as a function of wind speed (10 m height, m/sec) and water temperature (C). Two options are available. The first (and default) option is an equation by Wanninkhof et al. (1991):

$$k_a = \frac{0.464}{100\times3600} W_{10}^{1.61}\left(\frac{1447\,e^{-0.0537\,T}}{600}\right)^{0.5}$$

The second reaeration option is an equation by Chen and Kanwisher (1963):

$$k_a = \frac{2.4\times10^{-9}}{200 - 60\times W_{10}^{0.5}\times10^{-6}} \qquad for\ W_{10} < 10\ m/\sec$$

$$= \frac{2.4\times10^{-9}}{200 - 60\times10^{0.5}\times10^{-6}} \qquad for\ W_{10} \geq 10\ m/\sec$$

Values of k_a are adjusted to ambient water temperature using the "theta" temperature correction equation. Reaeration rate constant k_2 (m/day) is the quotient of the reaeration velocity and the surface layer depth:

$$k_2 = \frac{86400\,k_a}{d_s}$$

To conduct this test, set all advective flows, dispersion coefficients, and settling velocities to 0. Make sure that CBOD decay, nitrification, sediment oxygen demand, phytoplankton growth and respiration rate constants are set to 0. Specify temperature correction factor of 1.024 for reaeration, and values for wind speed, water temperature, and depth so that reaction doubling times are 1 day. Run the tests for the following range of conditions for each reaeration option:

- Water temperature: 10, 20, 30 C
- Wind speed: 5, 10, 20 m/sec
- Salinity: 20 PSU
- Initial DO Deficit: 5 mg/L

For salinity of 20, the calculated DO saturation concentrations should be:

- T = 10 C, DO_{sat} = 9.932876 mg/L
- T = 20 C, DO_{sat} = 8.080517 mg/L
- T = 30 C, DO_{sat} = 6.772362 mg/L

Model calculated values of DO saturation should be compared with these results. Initial DO concentrations should be specified to provide an initial DO deficit of 5 mg/L:

- T = 10 C, DO = 4.932876 mg/L
- T = 20 C, DO = 3.080517 mg/L
- T = 30 C, DO = 1.772362 mg/L

The two WQCBM reaeration equations produce the following reaeration velocities after temperature-correction and adjustment to units of m/day:

Table 23 – Wanninkhof et al. (1991) reaeration velocities

Wind Speed	Wanninkhof Reaeration Velocity, m/day		
m/sec	T = 10 C	T = 20 C	T = 30 C
5	1.396825	1.358481	1.321189
10	4.263834	4.146788	4.032954
20	13.015431	12.658145	12.310668

Table 24 – Chen & Kanwisher (1963) reaeration velocities

Wind Speed	Chen & Kanwisher Reaeration Velocity, m/day		
m/sec	T = 10 C	T = 20 C	T = 30 C
5	2.484634	3.149648	3.992654
10	15.938105	20.203948	25.611547
20	15.938105	20.203948	25.611547

Model calculated values of reaeration velocity should be compared with these results.

In order to produce a reaction rate with half-life of 1 day, the following depths must be specified:

Table 25 – Compartment depths for Wanninkhof et al. (1991) reaeration velocities

Wind Speed	Wanninkhof Reaeration Velocity, m/day		
m/sec	T = 10 C	T = 20 C	T = 30 C
5	2.015192	1.959873	1.906073
10	6.151412	5.982550	5.818323
20	18.777298	18.261844	17.760539

Table 26 – Compartment depths for Chen & Kanwisher (1963) reaeration velocities

Wind Speed	Chen & Kanwisher Reaeration Velocity, m/day		
m/sec	T = 10 C	T = 20 C	T = 30 C
5	3.584570	4.543982	5.760182
10	22.993825	29.148136	36.949652
20	22.993825	29.148136	36.949652

Run the simulation for duration 10 days (i.e., 10 half-lives) using each of the wind speeds and water temperatures. Check DO Deficit and DO concentrations to match the analytical solutions in Table 27.

Table 27 - Unit concentration response

Time	Concentration			
days	DO Deficit mg/L	DO (10 C) mg/L	DO (20 C) mg/L	DO (30 C) mg/L
0	5.000000	4.932876	3.080517	1.772362
1	2.500000	7.432876	5.580517	4.272362
2	1.250000	8.682876	6.830517	5.522362
3	0.625000	9.307876	7.455517	6.147362
4	0.312500	9.620376	7.768017	6.459862
5	0.156250	9.776626	7.924267	6.616112
6	0.078125	9.854751	8.002392	6.694237
10	0.004883	9.927993	8.075634	6.767479

Run the tests for the Wanninkhof reaeration option, then repeat for the Chen and Kanwisher option.