CHAPRA

Surface Water Quality Modeling

Example Problem 33-2

D0095

$$\overline{S} = \frac{\left(k_d + k_r + \frac{Q}{V}\right)k_s}{k_{g,\max} - \left(k_d + k_r + \frac{Q}{V}\right)} \tag{32.16}$$

and

$$\overline{X} = \frac{\frac{Q}{V}(S_{\text{in}} - \overline{S})}{\frac{1}{Y}k_g - k_d} \tag{32.17}$$

where $\overline{S}$ and $\overline{X}$ = steady-state concentrations of the substrate and bacteria, respectively, and k_g is defined by Eq. 32.2 with $S = \overline{S}$. Thus the ultimate steady-state substrate concentration is independent of the inflow concentration. In contrast the steady-state bacterial concentration varies directly with the inflow concentration.

EXAMPLE 32.4. WASHOUT RESIDENCE TIME AND ULTIMATE SUBSTRATE CONCENTRATION. (*a*) Determine $\tau_{\min}$ for the reactor from Example 32.3. (*b*) Calculate the steady-state substrate level for Example 32.3 with $\tau_w = 20$ hr.

Solution: (*a*) Equation 32.15 yields

$$\tau_{\min} = \frac{150 + 1000}{(0.2 - 0.01 - 0.01)1000 - (0.01 + 0.01)150} = 6.5 \text{ hr}$$

(*b*) Equation 32.16 gives

$$\overline{S} = \frac{(0.01 + 0.01 + 0.05)1.50}{0.2 - (0.01 + 0.01 + 0.05)} = 80.77 \text{ mgC L}^{-1}$$

which corresponds to the numerical result (Fig. 32.7*a*).

32.5 ALGAL GROWTH ON A LIMITING NUTRIENT

The theory of the previous sections can be easily extended to the growth of algae as a function of a limiting nutrient. A CSTR is depicted in Fig. 32.8 for the case of algae and the nutrient phosphorus. Mass balances can be written as

$$\frac{da}{dt} = \left(k_{g,\max}\frac{p}{k_{sp} + p} - k_d - \frac{Q}{V}\right)a \tag{32.18}$$

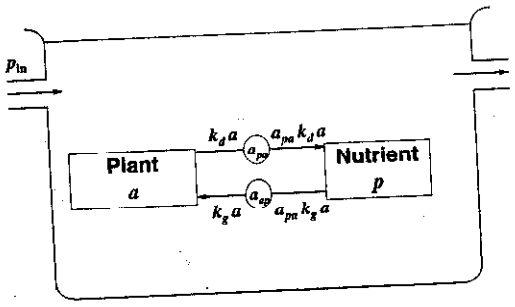

FIGURE 32.8
Flow diagram for kinetic interactions between plants and a limiting nutrient in a CSTR.

$$\frac{dp}{dt} = -a_{pa}k_{g,\max}\frac{p}{k_{sp}+p}a + a_{pa}k_d a + \frac{Q}{V}(p_{in} - p) \qquad (32.19)$$

where a and p = concentration of plants ("a" stands for "algae") (mgChl$a$ m^{-3}) and phosphorus (mgP m^3), respectively
k_{sp} = half-saturation constant for phosphorus (mgP m^{-3})
a_{pa} = ratio of phosphorus to chlorophyll a in algae (mgP mgChla^{-1})

Two important distinctions can be made between this scheme and the one for microbial decomposition from Fig. 32.6:

- Because the plants and the nutrient are measured on a different basis, stoichiometric conversions must be applied to transfers between the compartments.
- There is no loss of mass due to degradation processes as was the case for carbon. Thus the stoichiometric conversions do not involve a loss of mass, merely a change of units.

EXAMPLE 32.5. ALGAL/NUTRIENT INTERACTIONS. The epilimnion of a lake has the following characteristics at the beginning of the stratified period:

$a_0 = 0.5$ mgChl$a$ m^{-3}
$p_{in} = 10$ mgP m^{-3}
$k_{g,\max} = 1$ d^{-1}
$k_d = 0.1$ d^{-1}
$p_0 = 9.5$ mgP m^{-3}
$a_{pa} = 1.5$ mgP mgChla^{-1}
$k_s = 2$ mgP m^{-3}
$\tau_w = 30$ d

Assuming that mass transfer across the thermocline due to diffusion and settling is negligible, (*a*) simulate how the algae and phosphorus change over time, (*b*) calculate the ultimate, steady-state level of phosphorus, and (*c*) determine $\tau_{\min}$.

Solution: (*a*) The parameters can be substituted into Eqs. 32.18 and 32.19 and solved numerically with the fourth-order Runge-Kutta method. The results are displayed graphically in Fig. 32.9. The algae grow to a peak of 6.6 mg m^{-3} in about 4 d.

(*b*)

$$\overline{S} = \frac{[k_d + (Q/V)]k_s}{k_{g,\max} - [k_d + (Q/V)]} = \frac{[0.1 + 1/30]2}{1 - [0.1 + (1/30)]} = 0.308 \text{ mgP m}^{-3}$$

(*c*)

$$\tau_{\min} = \frac{k_s + p_{in}}{(k_{g,\max} - k_d)p_{in} - k_d(k_s)} = \frac{2 + 10}{(1 - 0.1)10 - 0.1(2)} = 1.36 \text{ d}$$

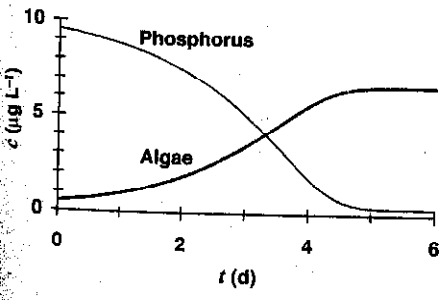

FIGURE 32.9
Flow diagram for kinetic interactions between plants and a limiting nutrient in a CSTR.

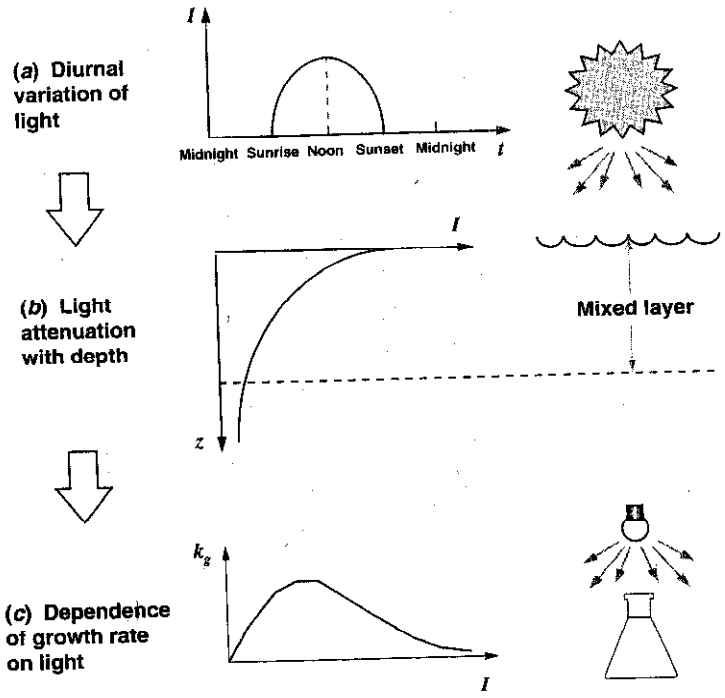

FIGURE 33.6
Incorporating light into the phytoplankton growth model involves integrating three separate factors: (*a*) the temporal variation of solar radiation at the water surface, (*b*) the attenuation of light as it passes through the layer of water being modeled, and (*c*) the effect of the light on plankton growth.

of models have been developed to fit light dependence. For example a Michaelis-Menten formulation is sometimes used,

$$F(I) = \frac{I}{k_{si} + I} \tag{33.18}$$

where k_{si} = a half-saturation constant for light (ly d^{-1}). Thus, as for nutrient limitation, this relationship is linearly proportional to light intensity at low light levels and constant at high levels. Consequently it does not capture growth attenuation at high light intensity. As was the case for Eq. 33.6 for temperature, such a formulation might be justified when the phytoplankton was simulated as a single group. In such cases it would be implicitly assumed that (1) some species of phytoplankton would grow optimally at any particular range of light intensity and (2) increasing light always leads to increasing growth. It would also be appropriate for a single species when the experiments were conducted below the optimal light intensity.

A somewhat different approach was taken by Steele (1965), whose model acknowledges that growth is inhibited at high light levels,

$$F(I) = \frac{I}{I_s} e^{-\frac{I}{I_s}+1} \tag{33.19}$$

where I = light level and I_s = optimal light level. Note that I_s ranges from about 100 to 400 ly d^{-1}. Lower values are appropriate for low-light-adapted species, whereas high values are for those that are adapted to high light intensity.

The temporal variation in light can be characterized by a half-sinusoid. For such cases the average light over the daylight hours can be computed as (Eq. 24.11)

$$I_a = I_m\left(\frac{2}{\pi}\right) \tag{33.20}$$

where I_m = maximum light intensity and f = photoperiod (sunlight fraction of day). Thus the average daylight value is about $\frac{2}{3}$ of the maximum.

The spatial variation of light down through the water column can be modeled by the Beer-Lambert law,

$$I(z) = I_0 e^{-k_e z} \tag{33.21}$$

where I_0 = solar radiation at the surface and k_e = extinction coefficient. The latter can be related to more fundamental quantities by (Riley 1956)

$$k_e = k_e' + 0.0088a + 0.054a^{2/3} \tag{33.22}$$

where k_e' = light extinction due to factors other than phytoplankton, which can be either measured directly or calculated via (Di Toro 1978),

$$k_e' = k_{ew} + 0.052N + 0.174D \tag{33.23}$$

where k_{ew} = light extinction due to particle-free water and color (m^{-1})
N = nonvolatile suspended solids (mg L^{-1})
D = detritus (nonliving organic suspended solids) (mg L^{-1})

All the preceding formulas can be applied to compute the mean light limitation for a well-mixed layer (Fig. 33.7). For example using the Steele model, we first substitute Eq. 33.21 into Eq. 33.19 to give an equation for the growth limitation at depth z,

$$F(I) = \frac{I_a e^{-k_e z}}{I_s} e^{-\frac{I_a e^{-k_e z}}{I_s}+1} \tag{33.24}$$

This function can then be integrated over depth and time to develop the mean value

$$\phi_L = \frac{1}{H}\int_{H_1}^{H_2}\frac{1}{T_p}\int_0^{fT_p}\frac{I_a e^{-k_e z}}{I_s} e^{-\frac{I_a e^{-k_e z}}{I_s}+1}\,dt\,dz \tag{33.25}$$

Evaluating this double integral results in

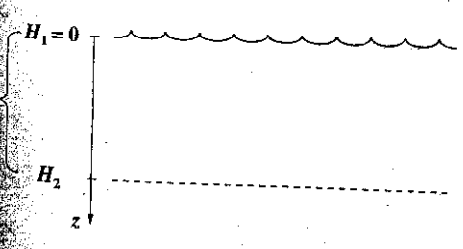

FIGURE 33.7
A layer of water of thickness $H = H_2 - H_1$. For this particular case, the surface layer is depicted ($H_1 = 0$).

$$\phi_L = \frac{2.718f}{k_e H}\left(e^{-\alpha_1} - e^{-\alpha_0}\right) \tag{33.26}$$

where

$$\alpha_0 = \frac{I_a}{I_s} e^{-k_e H_1} \tag{33.27}$$

and

$$\alpha_1 = \frac{I_a}{I_s} e^{-k_e H_2} \tag{33.28}$$

It should be noted that the light values used in all the preceding equations is visible, photosynthetically available light. This value is typically about 40 to 50% of the energy in the complete standard spectrum used for such calculations as heat budgets (Lec. 30) or photolysis (Lec. 42). For example Bannister (1974) and Stefan et al. (1983) suggest values from 44 to 46%. It should be noted that almost all the radiation outside the visible range is absorbed in the first meter below the surface (Orlob 1977).

33.5 THE GROWTH-RATE MODEL

The complete model of phytoplankton growth can now be developed as

$$k_g = k_{g,20} 1.066^{T-20} \left[\frac{2.718f}{k_e H}\left(e^{-\alpha_1} - e^{-\alpha_0}\right)\right] \min\left(\frac{n}{k_{sn}+n}, \frac{p}{k_{sp}+p}\right) \tag{33.29}$$

Temperature Light Nutrients

This formula has a variety of applications. In a later lecture we use it to calculate phytoplankton growth as part of a nutrient/food-chain model. In addition it can be employed to calculate some other quantities of interest to water-quality modelers. For example if the quantity of phytoplankton is known, it can be used to compute the primary production,

$$Pr = a_{ca} k_g H a$$

with units of gC m^{-2} d^{-1}, or the oxygen produced by photosynthesis,

$$P = r_{oc} a_{ca} k_g a$$

with units of gO m^{-2} d^{-1}. Finally it can be used to gain insight into which factors are limiting phytoplankton growth. All these applications are explored in the following example.

EXAMPLE 33.1. PHYTOPLANKTON GROWTH RATE. The epilimnion of a lake has the following parameters:

$T = 20°C$
$I_s = 300$ ly d^{-1}
Available P concentration = 3 mg m^{-3}
Available N concentration = 20 mg m^{-3}
Chlorophyll a concentration = 4 mg m^{-3}
$k_{g,20} = 2\ d^{-1}$
$I_a = 500$ ly d^{-1}
$k'_e = 0.3\ m^{-1}$
P half-saturation constant = 2 mg/l
N half-saturation constant = 10 mg/l
$f = 0.5$
$H = 5$ m

(*a*) Compute the phytoplankton growth rate. Assume that the suspended solids concentration (other than phytoplankton) is negligible.
(*b*) Determine the primary production rate in g m^{-2} d^{-1} if the chlorophyll-to-carbon ratio is 20 μgChl*a* mgC^{-1}.

Solution: (*a*) The extinction coefficient can be determined by

$$k_e = 0.3 + 0.0088(4) + 0.54(4)^{2/3} = 0.471 \text{ m}^{-1}$$

which can used in conjunction with the light data to calculate

$$\alpha_0 = \frac{500}{300} e^{-0.471(0)} = 1.667$$

and

$$\alpha_1 = \frac{500}{300} e^{-0.471(5)} = 0.158$$

which can be substituted into Eq. 33.29 to give

$$k_g = 2 \cdot 1.066^{25-20} \left[\frac{2.718(0.5)}{0.471(5)}\left(e^{-1.667} - e^{-0.158}\right)\right] \min\left(\frac{20}{10+20}, \frac{3}{2+3}\right)$$

$$2.753 \quad \times \quad 0.3838 \quad \times \quad 0.6 \quad = 0.634 \text{ d}^{-1}$$

Thus we can see that the temperature sets the maximum rate, whereas the light and nutrients diminish the ultimate value. Further, the equation indicates that phosphorus is the limiting nutrient.
(*b*) The rate can be translated into a daily primary production rate by

$$Pr = a_{cu} k_g H a$$

Substituting values gives

$$Pr = \frac{1 \text{ mgC}}{20\ \mu\text{gChl}a}\left(\frac{0.634}{\text{d}}\right)(5\text{m})\left(4\frac{\mu\text{gChl}a}{L}\right)\left(\frac{1 \text{ g}}{1000 \text{ mg}}\right)\left(\frac{1000 \text{ L}}{\text{m}^3}\right) = 0.634 \text{ gC m}^{-2} \text{ d}^{-1}$$

33.6 NONPREDATORY LOSSES

A number of processes contribute to the loss rate of phytoplankton in Eq. 33.3. In water-quality modeling, three losses are emphasized:

- *Respiration.* This refers to the process opposite to photosynthesis, where the plant utilizes oxygen and releases carbon dioxide.
- *Excretion.* This process has traditionally focused on the release of nutrients. However, algae can also release organic carbon as extracellular byproducts.
- *Predatory losses.* Death of algae due to grazing by zooplankton.

Because the first two processes are difficult to measure separately, they have usually been modeled as a single first-order decay. Thus the death rate from Eq. 33.3 is usually expanded, as in

$$k_d = k_{ra} + k_{gz} \tag{33.30}$$

where k_{ra} = loss due to the combined effects of respiration and excretion (d^{-1}), and k_{gz} = grazing losses (d^{-1}). Values for k_{ra} range between 0.01 and 0.5 d^{-1}, with typical values on the order of 0.1 to 0.2 d^{-1}. A theta model is usually used to correct the respiration/excretion rate for temperature. A value of $\theta = 1.08$, connoting a strong temperature effect, is conventional.

It should be noted that although they are often treated as a single process, the division between respiration and excretion should not be considered a trivial distinction. This is particularly true as nutrient/food-chain models evolve toward a more accurate representation of the organic carbon cycle. In such cases, processes that tend to generate carbon dioxide and liberate available nutrients (respiration) should be separated from processes that liberate organic forms of carbon and nutrients (excretion).

At this point we can now integrate the growth and decay mechanisms into our modeling framework. In an analogous fashion to Eqs. 32.18 and 32.19, we can develop the following mass-balance equations for a limiting nutrient and algae for a CSTR:

$$\frac{da}{dt} = \left[k_{g,T}\frac{p}{k_{sp}+p}\frac{2.718f}{k_eH}\left(e^{-\alpha_1}-e^{-\alpha_0}\right) - k_{ra} - \frac{Q}{V}\right]a \tag{33.31}$$

$$\frac{dp}{dt} = -a_{pa}k_{g,T}\frac{p}{k_{sp}+p}\frac{2.718f}{k_eH}\left(e^{-\alpha_1}-e^{-\alpha_0}\right)a + a_{pa}k_{r,a}a + \frac{Q}{V}\left(p_{in}-p\right) \tag{33.32}$$

Notice that we have omitted grazing losses, which will be described in more detail in the following lecture.

EXAMPLE 33.2. ALGAL/NUTRIENT INTERACTIONS WITH LIGHT LIMITATION. Perform the same calculation as in Example 32.5, but now include the effects of light limitation. Note that the epilimnion has the following characteristics at the beginning of the stratified period:

$a_0 = 0.5$ mgChl$a$ m^{-3}	$p_0 = 9.5$ mgP m^{-3}	$p_{in} = 10$ mgP m^{-3}
$a_{pa} = 1.5$ mgP mgChla^{-1}	$k_{g,T} = 1$ d^{-1}	$k_{sp} = 2$ mgP m^{-3}
$k_{ra} = 0.1$ d^{-1}	$\tau_w = 30$ d^{-1}	$f = 0.5$
$I_a = 400$ ly d^{-1}	$I_s = 250$ ly d^{-1}	$H = 10$ m
$k'_e = 0.1$ m^{-1}		

Assuming that mass transfer across the thermocline due to diffusion and settling is negligible, simulate how the algae and phosphorus change over time.

Solution: Using Eqs. 33.22 and 33.26 to quantify the light effect, we display the results graphically in Fig. 33.8. In contrast to Fig. 32.9, two major differences are evident. First, the final algae level is lower and the phosphorus higher for the present case. Second, the time to steady-state is longer when light limitation is included. Both are due to the reduction of algal growth from light limitation. Thus, because the growth rate is smaller, the final partitioning between plants and nutrient is less extreme. Similarly, the response time is lengthened.

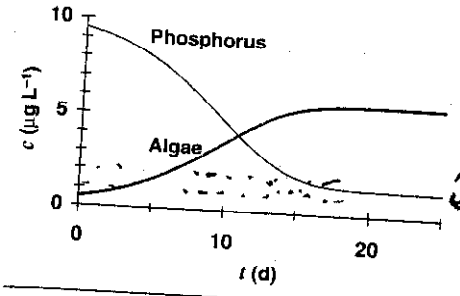

FIGURE 33.8
Flow diagram for kinetic interactions between plants and a limiting nutrient in a CSTR.

33.7 VARIABLE CHLOROPHYLL MODELS (ADVANCED TOPIC)

As described to this point, most water-quality models have used a constant stoichiometry to characterize algal concentration. An easy-to-measure quantity such as chlorophyll *a* was usually adopted as the measure of algal biomass. Transfers between phytoplankton and other model state variables such as nutrient pools were then handled by simple stoichiometric conversion factors.

Although this has proved to be a good first approximation, it has long been understood by ***phycologists*** (scientists who study algae) that cell stoichiometry is not constant. We have already alluded to this in our earlier discussion of luxury uptake. Beyond nutrients, a more fundamental issue relates to carbon and chlorophyll. In particular, the chlorophyll-to-carbon ratio is not constant, but varies in response to light levels and the physiological state of the cells. Reviews of the published literature (e.g., Bowie et al. 1985) indicate that the chlorophyll-to-carbon ratio varies between about 10 and 100 μgChl*a* mgC^{-1}.

There are two reasons why such variability could have significance in the coming years:

- The focus of modeling is shifting from nutrient/food-chain interactions to an organic carbon cycle characterization. This is due to the application of water-quality frameworks beyond eutrophication to encompass problems such as toxic pollution, sediment-water interactions, and the impact of disinfection byproducts on drinking water.
- Water-quality models are being increasingly used to analyze cleaner systems than were studied in the past. Many water bodies are cleaner because their loadings have been reduced through waste treatment. Further, new problems such as drinking-water quality are being addressed. Because heavily polluted systems are more turbid and dimly illuminated, they tend to have a more constant chlorophyll-to-carbon ratio. In contrast clean water bodies typically exhibit more variable light levels because significant light can penetrate beyond well-mixed surface layers. The existence of deep chlorophyll layers in some estuarine systems and clear lakes provides circumstantial evidence for such effects.

Over the past decade a number of models have been developed to account for variable chlorophyll content in plants. Today the models are beginning to be integrated into water-quality frameworks. The purpose of this section is to illustrate how such integration can be done.