MODELLING WATER QUALITY

Simple River Model

DO is one of the most important constituents of natural water systems; as fish and other aquatic animal species require oxygen.

Stream must have a minimum of 2 mg/L DO to maintain higher life forms, while most game fish require 4 mg/L.

Oxygen also important to maintain an aerobic state as the end products of chemical and biochemical reactions in anaerobic systems produce aesthetically displeasing odours, colours and taste.

When biodegradable organics are discharged into a stream, microorganisms convert the organics into new cells and oxidized waste products. During this process, DO is consumed.

The rate and quantity of DO consumption is dependent on the quantity of organics and the dilution capacity of the stream.

To replace the oxygen consumed, two mechanisms are relied on:

1. reaeration of oxygen from the atmosphere
2. production of oxygen by algal photosynthesis

Reaeration:

- the equilibrium concentration (saturation) of oxygen in the water is a function of temperature, salinity and pressure (values in back of text)
- if the dissolved concentration drops below the equilibrium value, there is oxygen transfer from the atmosphere into the water
- the difference between the equilibrium concentration and the actual concentration is called oxygen deficit and is expressed by:

$$D_t = C_s - C$$

where

- $D$ = dissolved oxygen deficit at any time $t$, mg/L
- $C_s$ = equilibrium DO concentration (saturation), mg/L
- $C$ = the actual oxygen concentration at any time $t$, mg/L

- $C_s$ does not change for the given conditions
\[ \frac{dD}{dt} = -\frac{dC}{dt} \] (1)

- deficit increases as DO is consumed and the rate of change can be expressed by:
- the oxygen deficit is the driving force for reaeration, greater the deficit, greater the rate of reaeration
- since reaeration is a first order rate equation, as expressed earlier in course:

\[ r_R = \frac{dC}{dt} = K(A/V)(C_s - C) \]

where

- \( r_R \) = rate of reaeration, \( g/m^3 \cdot d \)
- \( K \) = overall mass transfer coefficient, \( m/d \)
- \( A \) = surface area, \( m^2 \)
- \( V \) = liquid volume, \( m^3 \)

- for simplification,

\[ k_2 = K(A/V) \]

where, \( k_2 \) is reaeration constant, \( 1/d \), giving,

\[ r_R = k_2(C_s - C) \]

- factors affecting \( k_2 \) include
  - stream turbulence
  - surface area
  - water depth
  - temperature
    - temperature corrections are made by the same relationship used for BOD rate constant, except that \( \Theta = 1.024 \)

- typical values for \( k_2 \) at 20 °C, \( 1/d \) (base e) are as follows:

  - small ponds and back water \( 0.10 - 0.23 \)
  - sluggish streams and large lakes \( 0.23 - 0.35 \)
  - large streams with low velocity \( 0.35 - 0.46 \)
  - large streams at normal velocity \( 0.46 - 0.69 \)
  - swift streams \( 0.69 - 1.15 \)
  - rapids and waterfalls \( > 1.15 \)
Algal Photosynthesis

- in the presence of sunlight, algae metabolize inorganic compounds and produce oxygen
  \[
  CO_2 + 2H_2O \xrightarrow{\text{light}} CH_2O + O_2 + H_2 + \text{(new cells)}
  \]
- oxygen released is available to replenish the depleted DO
- as discussed earlier, excessive nutrients and sunlight can produce very active algae, which may produce so much O\_2 that the water becomes supersaturated; C>C_s
- however, the adverse affects of excessive algal growth outweigh the benefits of higher O\_2 production
- bacteria metabolism usually occurs downstream from where the oxygen is required
- also in absence of light, the algae obtain the energy from endogenous catabolism
  \[
  CH_2O + O_2 \rightarrow CO_2 + H_2O
  \]
  thus, the reaction contributes to oxygen demand rather than the supply
- since the excess oxygen (higher than saturation) can not be stored, it is released into the atmosphere.
  - occurs around 2 to 4 pm when the sunlight is high
  - after this point, the oxygen consumption begins to increase, resulting in reduced DO content, with the lowest levels occurring just before sunrise
  - has happen in areas of high algae growth, to such an extent that fish kills occur and odours occur
- due to variability of photosynthetically produced oxygen and the efforts made on minimum nutrient discharge, reaeration is considered as the only source of DO

Benthic Demand

- DO also affected by benthic demand, i.e., O\_2 uptake (deoxygentation) by sludge deposits
- typical benthic oxygen demand rates (r_B)
  - filamentous bacteria @ 10 g/m\^3 \( \sim 7 \text{ g/m}^2\text{•d} \)
  - municipal sewage sludge @ outfall \( \sim 4 \text{ g/m}^2\text{•d} \)
  - aged municipal sewage sludge @ outfall \( \sim 1.5 \text{ g/m}^2\text{•d} \)
  - estuarine mud \( \sim 1.5 \text{ g/m}^2\text{•d} \)
  - sandy bottom \( \sim 0.5 \text{ g/m}^2\text{•d} \)
  - mineral soils \( \sim 0.07 \text{ g/m}^2\text{•d} \)
Oxygen Sag Model

One of the earliest mathematical water quality models was developed by for the Ohio River by H.S. Streeter and E.B. Phelps in 1925. Hence the model is referred to as the Streeter-Phelps model.

Model relates the rate of change of the oxygen deficit with distance to the spatial rates of oxygen consumption and reoxygenation. Also referred to oxygen-sag model.

![Figure 1: OXYGEN SAG](image)

The change in oxygen with a river can be modelled by assuming the river is essentially a plug-flow reactor, where
Applying a mass balance to Figure 2 (Figure 8.2 in text) for the oxygen concentration in the stream, relating oxygen consumption to BOD and reoxygenation to natural reaeration, and neglecting hydrodynamic dispersion:

Accumulation = Inflow - Outflow + Deoxygenation + Reoxygenation

\[
\frac{\partial C}{\partial t}(\Delta V) = Q_{C_s} - Q_{C_s + \Delta x} + r_{\text{BOD}}(\Delta V) + r_{R}(\Delta V)
\]

(1)

where \( C \) is the \( O_2 \) concentration

substituting for \( r_{\text{BOD}} \) and \( r_{R} \) and taking the limit as \( \Delta x \) approaches zero

\[
\frac{\partial C}{\partial t} = -Q \frac{\partial C}{\partial V} - kL + k_2(C_s - C)
\]

(2)

where \( L \) is organic matter present at any time, (equal to \( \text{BOD}_{u(t)} \))

Assuming steady state conditions, \( \frac{\partial C}{\partial t} = 0 \), Eq. 2 becomes,

\[
QdC/dV = -kL + k_2(C_s - C)
\]

(3)

Assuming that the stream has a constant cross-sectional area, volume of reach is:

\[
V = Ax
\]

(4)

where \( x \) is the distance downstream, giving

\[
dV = Adx
\]

(5)
Since, \( x=ut \), with \( u \) being constant stream velocity and \( t \) residence time in stream

\[
dx = udt \quad (6)
\]
or

\[
dV = A \, dt \quad (7)
\]

Substituting Eq. 7 into Eq. 3 and rearranging gives

\[
Q \frac{dC}{A \, dt} = -kL + k_2(C_s - C) \quad (8)
\]
or

\[
\frac{dC}{dt} = -kL + k_2(C_s - C) \quad (9)
\]

Since,

\[
D_{(t)} = C_s - C_{(t)} \quad (10)
\]

the change in oxygen deficit with residence time is:

\[
dD/dt = -dC/dt \quad (11)
\]

Knowing that

\[
dC/dt = -kL + k_2(C_s - C) \quad (12)
\]
gives

\[
dD/dt + k_2D = kL \quad (13)
\]
or

\[
\frac{dD}{dt} + k_2D = kBOD_{w(0)} e^{-t} \quad (14)
\]

Comparison of Eq. 14 to a first order differential equation of the form \( dy/dx + Py = Q \), where \( P \) and \( Q \) are functions of \( x \), shows similarity. The use of an integrating factor is necessary.

For the oxygen deficit equation, the integrating factor is:
Thus multiplying both sides of the oxygen deficit equation (14) with the integrating factor (15) gives:

$$e^{k_2 t} \frac{dD}{dt} + k_2 D e^{k_2 t} = kBOD_{w(0)} e^{(k_2 - k)t}$$  \hspace{1cm} (16)

Since the left side of Eq. 16 can be factored as:

$$e^{k_2 t} \frac{dD}{dt} + k_2 D e^{k_2 t} = \frac{d}{dt} D e^{k_2 t}$$  \hspace{1cm} (17)

which leads to

$$\frac{d}{dt} D e^{k_2 t} = kBOD_{w(0)} e^{(k_2 - k)t}$$  \hspace{1cm} (18)

Separating variables and integrating gives

$$D e^{k_2 t} = \left( \frac{kBOD_{w(0)}}{k_2 - k} \right) e^{(k_2 - k)t} + K$$  \hspace{1cm} (19)

The constant of integration is determined from known boundary conditions, that is $D = D_i$ at $t=0$. Thus,

$$K = D_i - \frac{kBOD_{w(0)}}{k_2 - k}$$  \hspace{1cm} (20)

giving

$$D(t) = \left( \frac{kBOD_{w(0)}}{k_2 - k} \right) \left( e^{-k_2 t} - e^{-k t} \right) + D_i e^{-k_2 t}$$  \hspace{1cm} (21)

where, $D(t)$ is the oxygen deficit at any place along the stream
Note: t is the residence time in the stream, or in other words for constant flow and velocity;

\[ t = \frac{x \text{ (distance downstream)}}{u \text{ (stream velocity)}} \]  \hspace{1cm} (22)

**CRITICAL DEFICIT**

The critical point on the oxygen sag curve is called the *critical deficit, \( D_c \)*. This point (see Figure 1) has the lowest dissolved oxygen content and will determine the impact on living organisms in the stream.

The value for \( D_c \) can be determined by setting \( \frac{dD_c}{dt} = 0 \) (rate of change in deficit is zero) in Eq. 14, giving,

\[ 0 + k_2 D_c = kBOD_{w(0)} e^{-k_2 t} \]  \hspace{1cm} (23)

or

\[ D_c = \left( \frac{k}{k_2} \right) BOD_{w(0)} e^{-k_2 t} \]  \hspace{1cm} (24)

To find \( D_c \), a value for \( t_c \) is required. This can be determined by differentiating the deficit equation (21), as \( \frac{dD_c}{dt} = 0 \) at maximum \( t_c \). This gives:

\[ 0 = \left( \frac{kBOD_{w(0)}}{k_2 - k} \right) (-k_2 e^{-k_2 t_c} + k_2 e^{-k_2 t_c}) - k_2 D_c e^{-k_2 t_c} \]  \hspace{1cm} (25)

rearranging and simplifying gives,

\[ t_c = \left( \frac{1}{k_2 - k} \right) \ln \left[ \frac{k_2}{k} \left( 1 - D_c \frac{k}{k_2 - k} \right) \frac{k_2}{k} \right] \]  \hspace{1cm} (26)

**BENTHIC DEMAND**

When benthic demand is included, deficit (g/m³) can be expressed as:

\[ D_{b(0)} = \left( \frac{kBOD_{w(0)}}{k_2 - k} \right) \left( e^{-k_2 t} - e^{-k_2 t_c} \right) + D_c e^{-k_2 t} + \frac{r_B}{k_2} (1 - e^{-k_2 t}) \]  \hspace{1cm} (27)
where, \( r_B \) is zero order uptake rate (g/m³), given by \( r_B^* \) (g/m²) divided by average stream depth (m)

\[
    r_B = \frac{r_B^*}{d}
\]  

(28)

Corresponding Critical Deficit (\( D_{CB(0)} \)) is:

\[
    D_{CB(0)} = \left( \frac{k \text{BOD}_u(0)}{k_2} \right) e^{-k_2 t_m} + \frac{r_B}{k_2}
\]  

(29)

and time to critical deficit (\( t_{nc} \)),

\[
    t_{nc} = \left( \frac{1}{k_2 - k} \right) \ln \left[ \frac{k_2}{k} - \frac{k_2 D_i (k_2 - k) + r_B (k_2 - k)}{k^2 \text{BOD}_u(0)} \right]
\]  

(30)

Comments

- position of critical deficit is related to system variables \( k \), \( k_2 \), \( \text{BOD}_{uo} \), \( D_i \) and \( u \)
- time of travel to \( t_i \) is influenced by \( k \) and \( k_2 \)
- magnitude of \( D_i \) influenced by \( \text{BOD}_{uo} \)
- heavy organic loading result in large oxygen deficits, which may turn stream anaerobic; since anaerobic metabolism is a slow process and recovery long, oxygen sag is extended farther downstream
- Improving DO
  - build municipal water falls; Illinois along the Calumet Waterway System
    - 5 such stations added 50,000 lbs of O₂ to the river WQI 1991(4), pg. 36
    - is a form of advanced wastewater treatment (tertiary)