Vol. 7, Issue 4, April 2018,

ISSN: 2320-0294 Impact Factor: 6.765

Journal Homepage: http://www.ijesm.co.in, Email: ijesmj@gmail.com

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Peer Reviewed Refereed Open Access International Journal - Included in the International Serial Directories Indexed & Listed at: Ulrich's Periodicals Directory ©, U.S.A., Open J-Gage as well as in Cabell's Directories of Publishing Opportunities, U.S.A

MATHEMATICAL INTRODUCTION OF SEDIMENT OXYGEN DEMAND, PHOTOSYNTHESIS & RESPIRATION AND SOLIDS DEPOSITION PROCESSES

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Abstract

Keywords:

Sediment oxygen demand;
Dissolved Oxygen;
Solids Deposition;
Photosynthesis & Respiration.

this paper we have presented mathematical introduction of Sediment Oxygen Demand, Photosynthesis & Respiration and Solids Deposition process as a transformation process, these process are very important in the study of water quality, which are constituent-specific, which affect all water quality parameters. The major factors affecting SOD are temperature, oxygen concentration at the sediment water interface (available oxygen), makeup of the biological community, organic and physical characteristics of the sediment, current velocity over the sediments, and chemistry of the interstitial water. In Photosynthesis & Respiration, the net algal oxygen production minus consumption is simulated by QUAL-II, and in solid deposition process, settling is enhanced by flocculation and hindered by ambient turbulence. In rivers and coastal areas, turbulence is often sufficient to distribute the suspended-solids over the entire water depth.

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Vol. 7, Issue 4, April 2018,

ISSN: 2320-0294 Impact Factor: 6.765

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1. Introduction

Water quality parameters are relating to waste water discharge are dissolved oxygen, suspended solids, bacteria, nutrients, PH and toxic chemicals including volatile organics, acid/base, neutrals, metals and pesticides. Biodegradation of organic matter in the sediment affect level of DO in the overlying water. Dissolved oxygen is important to aquatic life because detrimental effects can occur when DO levels drop below 4 to 5 mg/L, depending on the aquatic species. Suspended solids affect water column turbidity and ultimately settle to the bottom, leading to possible benthic enrichment, toxicity and sediment oxygen demand. Coliform bacteria are used as an indicator of other pathogenic organisms of fecal origin and as such provide a measure of the safety of the water for recreational and other uses. Nutrients can lead to eutrophication and DO depletion. The acidity of water, measured by its PH, affects the chemical and ecological balance of ambient waters. Toxic chemicals include arrange of compounds that, at different concentrations, have detrimental effects on aquatic life or on humans, upon ingestion of water and/or fish and shellfish.

Oxygen demand by benthic sediments and organisms can represent a large fraction of oxygen consumption in surface waters. Benthal deposits at any given location in an aquatic system are the result of the transportation and deposition of organic material. The material may be from a source outside the system such as leaf litter or wastewater particulate BOD (allochthonous material), or it may be generated inside the system as occurs with plant growth (autochthonous material). In either case, such organic matter can exert a high oxygen demand under some circumstances. In addition to oxygen demand caused by decay of organic matter, resident invertebrates can generate significant oxygen demand through respiration [31]. The importance of this process to water quality modeling is reflected in a recent symposium [14]. This same symposium also reviewed measurement techniques and a concensus favoring in situ measurement was reached.

In addition to nitrogen, other nutrients are needed for biomass growth, notably phosphorus and silica. The average molar ratios of nitrogen to phosphorus to carbon in algal protoplasm (Redfield ratios) are approximately N:P:C =15:1:105 [20]. If one of these nutrients is available in smaller proportion to the others, it tends to limit growth and any addition of this nutrient will result in a direct increase of biomass. For example, in lakes, phosphorus is typically the limiting nutrient so

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that addition of phosphorus will spur growth but addition of nitrogen will have minimal effect.

Determining the impact of photosynthesis and respiration on dissolved oxygen requires detailed analyses. One approach is to simulate the fate of limiting nutrient through an element cycle in which the different forms under which the element can be present are evaluated [21]. In this paper we discussed Mathematical modeling of Sediment oxygen demand, Mathematical modeling of Photosynthesis & Respiration and Mathematical modeling Solids Deposition transformation processes [15].

2. Modeling of Sediment Oxygen Demand (SOD)

The process is usually referred to as sediment oxygen demand (SOD) because of the typical mode of measurement: enclosing the sediments in a chamber and measuring the change in dissolved oxygen concentration at several time increments. This technique is used in the laboratory or in situ. The oxygen utilized per unit area and time $(gO_2/m^2/day)$ is the SOD. The technique measures oxygen consumption by all of the processes enclosed in the chamber: chemical reactions, bacterially mediated redox reactions, and respiration by higher organisms (e.g., benthic worms, insects, and molluscs). Background water column respiration is then subtracted from this rate to compute the component due solely to the sediment interface. SOD is usually assumed to encompass the flux of dissolved constituents such as DO to sediment and reduced chemicals to the water column. However, solid particle flux as BOD or sediment entrainment or settling is modeled separately.

The major factors affecting SOD are: temperature, oxygen concentration at the sediment water interface (available oxygen), makeup of the biological community, organic and physical characteristics of the sediment, current velocity over the sediments, and chemistry of the interstitial water. Each of these factors is a resultant of other interacting processes occurring elsewhere in the aquatic system. For example, temperature and available oxygen can be changed as a result of transport and biochemical processes in the water column or system boundaries. Temperature and oxygen are usually modeled explicitly, and can be used as input variables to the SOD process equations. Another important linkage is that the biological community will change with the water quality (e.g., oxygen and nutrient concentrations) and productivity of the system. The organic characteristics will change over the long term due to settling of organic matter (detritus, fecal matter, phytoplankton) and its subsequent degradation and/or burial by continued biological community and the organic and physical sedimentation. The characteristics of the bottom sediments are usually treated as a composite

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characteristic of the particular system. Recently, techniques have been developed for investigating these factors; however, the usual technique is to measure the SOD directly rather than the underlying factors that control the processes of SOD.

At least two major factors affecting SOD are usually neglected in SOD modeling. Current velocity is often neglected despite the fact that it has a major effect on the diffusive gradient of oxygen beginning just below the sediment-water interface. Most measurement techniques provide mixing by internal mixing or by recirculating or flow-through systems to minimize the

effect of concentration gradients. However, the velocity of such systems may be insufficient [33] or may be so vigorous as to cause scour and re-suspension. Interstitial water chemistry affects substrates for biochemical and non-biochemical oxidation-reduction reactions and their reaction rates. This factor is also usually neglected in SOD measurements and kinetic formulations.

2.1 Kinetics

The generalized equation for sediment oxygen demand is:

$$\frac{dC}{dt} = \frac{-\text{SOD}}{H} = f$$
 (dissolved oxygen,

temperature, organisms, substrate) (2.1.1)

Where H = water depth, m

SOD= sediment oxygen demand (as measured), $gO_2/m^2/day$

t = time

C = oxygen concentration in the overlying water, mg/l

2.2 Dissolved Oxygen

The benthic oxygen consumption has been hypothesized to depend on the dissolved oxygen concentration in the overlying waters [7, 18].

$$SOD = a C^b$$

where a, b =empirically determined constants. In the [18] study, b was found to be 0.30 and a to vary from 0.09 to 0.16, primarily as a function of the population density of benthic invertebrates. We use a Michaelis-Menten relationship to express the effects of oxygen on SOD:

$$\frac{dC}{dt} = -\frac{k_s A_s}{V} \frac{C}{K_{02} + C}$$

Where $k_s =$ rate constant for SOD in Lake Erie, 0.1 $g \ O_2/m^2/day$ $A_s =$ area of the sediment, m^2

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 $V = \text{volume of water layer, } m^3$

 K_{0_2} = oxygen half saturation constant (1.4 mg/l)

C = oxygen concentration, mg/l

We divided SOD in Hamilton Bay in Lake Ontario into two fractions: chemical-microbial (CSOD) and biological (BSOD) [1]. The chemical fraction was defined as a first-order function of oxygen:

$$CSOD = k_1(T)C$$

Where $k_1(T)$ =temperature-adjusted rate constant for biochemical SOD, I/day

The biological fraction was estimated to be 20-40 percent due to macro invertebrates in Hamilton Bay sediments but still followed a Michaelis-Menten relationship:

$$BSOD = u(T) \frac{C}{K_{0_2} + C}$$

Where u(T) = temperature-adjusted rate constant for biological SOD (Obtained by measurement: range = 0.58 to 5.52 g $O_2/m^2/day$). 1/day K_{O_2} = oxygen half-saturation constant $(1.4 \, mg/l)$

It is interesting to note the similarity between the two estimates of K_{0_2} . The direct effects of dissolved oxygen on the rate constant are generally neglected except in a few models. For example, in the HSPF model, dissolved oxygen concentration affects the rate of sediment oxygen utilization exponentially:

$$\frac{dC}{dt} = -\frac{k_T}{H} (1 - e^{-1.22 C})$$

Where

 k_T = temperature adjusted rate constant, mg/m^2 -day

2.3 Temperature

Temperature effects on SOD are most commonly modeled using the van't Hoff form of the Arrhenius relationship:

$$k_T = k_{Tr} \theta^{(T-Tr)}$$

(2.3.1)

Where

 k_T = the rate at ambient temperature T

 k_{Tr} = the rate at a reference temperature (usually Tr = 20°C)

 θ = the temperature coefficient for adjusting the rate

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Although this form of the relationship is the most common and gives equivalent results to the Arrhenius equation, it is not preferred in standard nomenclature [11].

The exceptions to use of Equation (2.3.1) are RECEIV-II [22], HSPF and SSAM-IV [12]. RECEIV-II apparently does not provide a temperature correction for the SOD rate coefficient although other rate coefficients in the model are adjusted according to Equation (2.3.1) with $\theta = 1.047$ for CBOD. HSPF uses a linear function for adjusting the SOD for temperature:

$$k_T = 0.05 T_w k_{20}$$

(2.3.2)

Where

 k_T = the temperature adjusted coefficient

 k_{20} = the rate constant at 20°c

 T_w = water temperature, 0c

2.4. Sediment oxygen demand in control volume

Sediment oxygen demand is rate at which dissolved oxygen is removed from the water column during the decomposition of organic matter in lakebed sediments. The solids discharged with treated wastewater are partly organic. Upon setting to the bottom, they decompose anaerobically as well as aerobically, depending on conditions. The oxygen consumed in aerobic decomposition represents another dissolved - oxygen sink for the water body. For a control volume in contact with the bottom, the rate of dissolved - oxygen depletion due to sediment oxygen demand is given by [3]

$$r_S = \frac{k_S}{H}$$

(2.4.1)

Where

 $r_{\rm S}$ = rate of oxygen consumption due to SOD per unit time per unit volume of water, M/TL³

 k_S = Sediment oxygen uptake rate, M/L²T

H=depth of control volume, L

The major factors affecting k_S are the organic content of the sediments, temperature, dissolved oxygen at the sediment-water interface, makeup of the biological community, and current speed [2].

Measurement of k_S can be accomplish using a flux chamber to isolate the sediments from the overlying water. Dissolved in the chamber is measured versus time, from which k_S can be determined. In <u>situ</u> measurements are preferable, but their reliability is often questionable because of spacial variability and because the bottom shear exerted by the flow is difficult to reproduce in the flux chamber. For

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preliminary analyses the following order of magnitude values can be used for k_S : 0.2-1.0 g/ft² d(2-10 g/m² d) in the vicinity of municipal wastewater outfalls; 0.1-0.2 g/ft² d (0.2-1 g/m² d) for areas downstream of municipal outfalls & natural estuarine mud; 0.02-0.1 g/ft² d(0.2-1 g/m² d) for sandy bottom; and 0.005-0.01 g/ft² d(0.05-0.1g/m² d) for mineral soils. The uptake rates k_S can also be estimated based on solids deposition rates by assuming that the rate of decomposition equals to that of deposition [28].

$$k_S = r_o a R_d$$

(2.4.2)

Where r_o = oxidizable organic content of discharged solids, typically 0.5 and 0.6 for secondary effluent and 0.8 for primary effluent

a=oxygen / sediment stoichiometric ratio=1.07

 R_d = solids deposition rate, M/L²T

3. Modeling of Photosynthesis & Respiration

Photosynthetic oxygen production (P) and respiration (R) can be important sources and sinks of dissolved oxygen in natural waters. Many models simulate these processes directly in terms of algal growth and respiration. For example, net algal growth is simulated with the QUAL-II model [23] using:

$$\frac{\partial A}{\partial t} = (\mu - \rho - \sigma)A$$

(3.1)

Where

A =algal concentration, mass/volume

 μ = specific growth rate of algae, 1/time

 ρ = algal respiration rate, 1/time

 σ = algal settling rate, 1/time

The net algal oxygen production minus consumption is simulated by QUAL-II as:

$$\frac{\partial \mathcal{C}}{\partial t} = (a_1 \mu - a_2 \rho) A$$

(3.2)

where C = dissolved oxygen concentration, mass/volume

 a_1 = oxygen production per unit of algal mass, mass oxygen/mass algae

 a_2 = oxygen uptake per unit of algal mass, mass oxygen/mass algae

The stoichiometric coefficients a_1 and a_2 relate algal growth and death to oxygen production and consumption. In addition to algal respiration, respiration from zooplankton and nekton can contribute to oxygen depletion, and would be included in Equation (3.2), along with additional equations to describe their growth and death. Here we describe methods to predict P-R without simulating algal

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growth or respiration. The methods pertain largely to streams and rivers, and are useful in that they simplify the modeling approach.

It should be mentioned that some water quality models do not simulate photosynthesis and algal respiration. This approach is valid where P=0 and R=0. Other models simulate only daily average photosynthetic oxygen production (\bar{P}) and daily average respiration (\bar{R}) . If, on a daily average basis, $\bar{P}-\bar{R}\approx 0$, these models would predict little effect of algal activity on dissolved oxygen. However, if \bar{P} and \bar{R} are both large numbers, then actual dissolved oxygen levels will be higher during the day and lower at night than predicted by the models.

3.1 Methods to predict time-varying P - R values and daily average values

Erdmann [8, 9] has developed methods to predict time-varying P-R values and daily average values. In the time varying case the concept of the Stokes total time derivative is used. The total derivative is the sum of the time derivative $(\partial C/\partial t)$ and the advective derivative $(U\partial C/\partial x)$. The time derivative is evaluated as the average of two times, and the advective derivative is the average between two stations.

Gulliver [13] provide a literature review of the various methods used to predict P-R in streams. They also developed a computerized model to determine P-R that includes dispersion. However, they found that effects of dispersion were negligible for their applications. We use a single station method to predict monthly average P-R values [24], and the work of Simonsen and Harremoes [25] who used a two station approach to predict P-R on a river in Denmark.

The final two methods are the light-dark bottle method and the benthic chamber method. These methods measure P-R of algae in the water column (light-dark bottles) and of attached algae (benthic chamber). The methods provide single point estimates that may not be representative of the water body as a whole. Some models simulate daily average photosynthetic oxygen production rather than time-varing production. Erdmann [9] shows that, the daily average photosynthesis oxygen products rates, P, can be approximated by:

$$\bar{P} = \frac{2\Delta DO}{24} \qquad (mg/$$

Where ΔDO =daily maximum dissolved oxygen concentration minus daily minimum dissolved oxygen concentration, $\frac{mg}{l}$.

This approximation appears to be valid only for reaeration rates less than 0.2/day

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Vol. 7, Issue 4, April 2018,

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[16]. A second method of estimating P is to integrate a sinusoidal curve that represents the instantaneous photosynthetic oxygen production rate. The result is:

$$\bar{P} = \frac{2P_m P}{\pi}$$

(3.1.2)

Where

 P_m = maximum daily photosynthetic oxygen production rate, mg/l/day

p =fraction of day when algae are producing oxygen, decimal fraction

The U.S. EPA [29] describes a third method to estimate daily average production based on light-dark bottle measurements:

$$\bar{P} = \frac{2P'\Delta T}{\cos(\pi t_1/f) - \cos(\pi t_2 f)}$$

(3.1.3)

Where

 $P^{'}=$ observed average production rate between times t_{2} and t_{1}

$$\Delta T = (t_2 - t_1)/24$$

f = number of hours in day when oxygen is being produced

Relationships between photosynthetic oxygen production and chlorophyll-a have been developed by a number of researchers. While a detailed review of these methods is outside of the scope of this section, several of the more commonly used formulations are summarized here.

Megard [19] developed the following expression for daily average photosynthetic oxygen production:

$$\bar{P} = \frac{\ln\left(\frac{I_0}{I_Z}\right)C_a P_m}{\varepsilon_c C_a + \varepsilon_w}$$

(3.1.4)

Where I_0 = light intensity at the water surface

 I_Z = light intensity at depth z

 C_a = chlorophyll-a concentration

 ε_c = specific attenuation of light by chlorophyll-a

 ε_w =specific attenuation of light by all causes other than chlorophyll-a

 P_m = maximum daily photosynthetic oxygen production rate, mg/l/day

Demetracopoulos and Stefan modified this expression to predict hourly photosynthetic oxygen production, and used the expression in a model of the Mississippi River [5].

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In experiments on the Sacramento-San Joaquin Estuary, Bailey correlated the daily photosynthetic oxygen production rate to a number of factors [1]. The resulting expression was:

$$P_{av} = 3.16 C_a \frac{I^{0.677}}{k_c} + 0.16T - 0.56H$$

(3.1.5)

Where P_{av} = average daily gross photosynthetic rate, mg/l/day

I = mean daily solar intensity, cal/sq.cm/day

 k_e = light extinction coefficient, l/meter

 $T = \text{mean temperature, } \circ c$

H = mean water depth, m

 C_a = mean chlorophyll, mg/l

Finally, simple relationships between chlorophyll-a and, P_m have been Proposed [29]. This shows Pm/Ca ratios are influenced by water temperature and algal carbon/Ca ratios. For a typical water temperature (20°c) and a typical carbon/Ca ratio (50), Pm/Ca = 0.25. However, this ratio is likely to vary between 0.1 to 0.6 for the range of conditions present in streams.

4. Modeling of Solids Deposition:

The suspended solids discharged with treated wastewater ultimately settle to the bottom of the receiving water body. This settling is enhanced by flocculation and hindered by ambient turbulence. In rivers and coastal areas, turbulence is often sufficient to distribute the suspended-solids over the entire water depth. The rate of decay of the suspended-solids concentration due to settling is given by [10].

$$r_D = \frac{w}{H}S$$

(4.1)

Where r_D =rate of deposition per unit time per unit volume of water,

$$M/T L^3$$

S=Suspended-solids concentration, M/L³

w=settling velocity of the solids, L/T

H=water depth (if vertically mixed) or depth of control volume, L

Because of the very low solids concentrations obtained after initial effluent mixing and because of ambient turbulence, settling velocities are very low and difficult to measure [4]. Typical settling velocities obtained from settling column tests are given in table 4.1 [26]. Holographic measurements indicate lower settling velocities with a median of less than 3.33 X 10^{-6} ft/s (for samples of blended primary / secondary effluent) [32].

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Table 4.1: Settling velocities of suspended solids in primary and secondary effluents [10]

Settling velocity		Percent of total	
ft/s	cm/s	Primary Secondary	
3.3×10^{-4} 3.3×10^{-5} $\leq 3.3 \times 10^{-6}$	10^{-2} 10^{-3} $\leq 10^{-4}$	20 16 30 34	
		50 50	

Results and Analysis

It is generally agreed [17] that the organic matter oxygen demand is influenced by two different phenomena. The first is the rate at which oxygen diffuses into the bottom sediments and is then consumed. The second is essentially the rate at which reduced organic substances are conveyed into the water column, and are then oxidized. Traditional measurement techniques, whether they are performed in situ or in the laboratory, do not differentiate between the two processes but measure, either directly or indirectly, the gross oxygen uptake. Hence, in modeling dissolved oxygen, a single term in the dissolved oxygen mass balance formulation is normally used for both processes. If the two phenomena are modeled separately [6], then additional modeling complexity is necessary.

Ambient DO levels can be affected by the growth of algae (phytoplankton, primary productivity) and weeds (macrophytes) feeding on ammonia and nitrate. In this context, these nitrogenous compounds are nutrients. Algae and weeds constitute an oxygen source during daylight hours due to photosynthesis and a continuous oxygen sink due to respiration. For moderate nutrient enrichment levels, photosynthesis and respiration tend to compensate for each other with small overall impact. Higher enrichment levels, however, lead to high productivity (a situation called "eutrophication") with potentially strong effects on DO. Diurnal fluctuations can develop with supersaturated DO levels during daylight hours due to photosynthesis and very low DO levels at night due to respiration. Longer term fluctuations result from photosynthesis/ respiration imbalances during high biomass growth and decay periods.

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Conclusion:

The major factors affecting Sediment oxygen uptake rate are the organic content of the sediments, temperature, dissolved oxygen at the sediment-water interface, makeup of the biological community, and current speed and very low solids concentrations obtained after initial effluent mixing and because of ambient turbulence, settling velocities are very low and difficult to measure. We describe methods to predict P-R without simulating algal growth or respiration. The methods pertain largely to streams and rivers, and are useful in that they simplify the modeling approach. It should be mentioned that some water quality models do not simulate photosynthesis and algal respiration. This approach is valid where P=0 and R=0. Other models simulate only daily average photosynthetic oxygen production (\bar{P}) and daily average respiration (\bar{R}) . If, on a daily average basis, $\bar{P} - \bar{R} \approx$ 0, these models would predict little effect of algal activity on dissolved oxygen. However, if \bar{P} and \bar{R} are both large numbers, then actual dissolved oxygen levels will be higher during the day and lower at night than predicted by the models. In rivers and coastal areas, turbulence is often sufficient to distribute the suspendedsolids over the entire water depth.

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Vol. 7, Issue 4, April 2018,

ISSN: 2320-0294 Impact Factor: 6.765

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