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Journal of Geographical Research
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ARTICLE

Prediction of Dissolved Oxygen and Study of Engineered Nanoparticles to Improve Water Quality

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ARTICLE INFO

Article history
Received: 12 June 2020
Accepted: 17 June 2020
Published Online: 30 June 2020

Keywords:
DO (Dissolved Oxygen)
BOD (Biological Oxygen Demand)
Aeration rate
Nanoparticles
EDTA
Chelates

ABSTRACT

The lack of fresh water is one of the greatest challenges of our time. Increasing population and arid regions due to the temperature change limit the use of clean water. In this paper, Streeter-Phelps equation was used to find the levels of DO(Dissolved Oxygen) and the oxygen deficit which are the main criteria for the water body quality. Reaeration constants and deoxygenation coefficients were used to find how the DO and BOD(Biological Oxygen Demand) of the water bodies converge to equilibrium. Some pollutants cannot be removed from water efficiently via traditional water treatment. EDTA derivatives, owing to their engineered chemical properties, are also studied to be the potential metal ion chelator for enhancement of water quality. These molecules were tested for their thermodynamic stabilities, reactivities, and polarizations, and these characteristics are found to be important factors in selecting the most suitable chelator for metal ion chelation which is used for water quality control.

1. Introduction

In the static and dynamic environment of the aquatic system, the main variables affecting aquatic conditions are BOD(Biological Oxygen Demand), DO(Dissolved Oxygen), pH, and so on. Thus, the overall condition of the aquatic system including water quality can be assessed by measuring those factors by experimental or theoretical methods [1].

Among those factors, the DO is the most important factor that determines the quality of a body of water. A stream is considered healthy if the DO exceeds 5 mg/L and most fish do not survive if the DO is below 5 mg/L [2].

Organic matter in water with the exception of pathogens is considered a pollutant even though it is generally not harmful. Oxygen is used up in the bacterial decomposition process.

The equation below shows L_0, or the resulting BOD of the river/wastewater mixture. “Q” represents flow and “L” represents the BOD of “$_r$”, the river water, or “$_w$”, the waste water.

$$L_0 = \frac{Q_r L_r + Q_w L_w}{Q_r + Q_w}$$

Where :
L_0 = Ultimate BOD at the point of waste discharge
Q_r = Flow in the river upstream of the discharge
L_r = Ultimate BOD of the river water
Q_w = Flow of waste water from the discharge
L_w = Ultimate BOD in the discharged waste water

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DOI: https://doi.org/10.30564/jgr.v3i2.1984

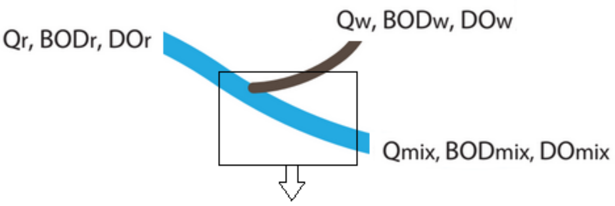

Figure 1. The DO and BOD of the river, wastewater and mixture

In the beginning, when the wastewater is first added to the river, there is some level of initial oxygen deficit in the wastewater. This results in a DO deficient in the stream. To determine this initial DO value, or DO_0, the L_0 formula can be used. Subtracting initial DO (DO_0) from DO_{sat} gives us D_0. This equation is shown below [3].

$$D_0 = DO_{sat} - DO_0$$

Now, when considering the downstream river and its DO, the following equation is examined. Here the rate of deficit increase is the difference of the rate of deoxygenation and the rate of reaeration.

At this point, the Streeter-Phelps curve formula can be derived :

$$D = \frac{k_d L_0}{k_r - k_d}\left(e^{-k_d t} - e^{-k_r t}\right) + D_0 e^{-k_r t}$$

where, the k_d is rate of deoxygenation and k_r is rate of reaeration [4].

A graph of DO and distance downstream can be developed using computation. At each point, the D is subtracted from D_o and the result is plotted on the graph.

Further examining the DO curve and oxygen deficiency, DO is initially consumed at a faster rate than it oxygen is reaerated from the atmosphere. The net DO of water is still dropping, which is why the curve also drops at this point. However, the system becomes more stable as time passes, as BOD decreases and the deoxygenation rate also decreases to roughly equal the reaeration rate. At this critical point, the DO reaches the minimum point and it increases downstream of the critical point.

2. Effect of Reaeration Constant of the Body of Water on the Dissolved Oxygen

Assume the sewage flown into a water body from the 38,000 people in a city is 50 cubic feet per second. The DO of the water body is 5.0mg/L and the BOD of the water body is 17.0 mg/L. They flow into a flowing water body that has a flow rate of 100 cfs and a flow speed of 1.0 ft/s. And other factors are:

(1) BOD in the creek upstream of the release point: 2.0mg/L

(2) DO in the creek upstream of the release point: 7.0 mg/L.

(3) The saturation value of DO: 9.0 mg/L.

(4) The deoxygenation coefficient k_1: 0.6/day

(5) The reaeration coefficient k_2: 0.3/day.

From the data above, we are finding:

(1) The initial oxygen deficit, BOD just downstream of the outfall

(2) The time and distance to reach the minimum DO

(3) The DO that could be expected 150 miles(or 150 days) downstream

Table 1. BOD, DO and other variables

Q (waste)	50 cfs	**Q (river)**	100 cfs	**DO sat**	9 mg/L
BOD (waste)	17 mg/L	**BOD (river)**	2 mg/L	**k_1**	0.6 1/day
DO (waste)	5 mg/L	**DO (river)**	7 mg/L	**k_2**	0.3 1/day

Equations for calculating DO and BOD at mixture: [5]

$$L_0 = \frac{Q_r L_r + Q_w L_w}{Q_r + Q_w}$$

$$(Q_r * DO_r) + (Q_w * DO_w) = (Q_m * DO_m)$$

$$D_o = DO_{sat} - DO_{mix}$$

Streeter-Phelps Equation:

$$D = \frac{k_1 L_a}{k_2 - k_1}(e^{-k_1 t} - e^{-k_2 t}) + D_a e^{-k_2 t}$$

Let's see how the reaeration constant of the body of water influences the dissolved oxygen, DO.

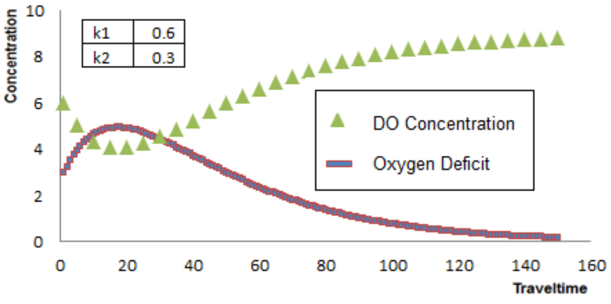

Figure 2. Changes of the DO and oxygen deficit for k_1=0.6 and k_2=0.3

Figure 2 displays a water system undergoing recovery

DOI: https://doi.org/10.30564/jgr.v3i2.1984

from organic pollution. The initial C_{DO} at 6.2 mg/L, far exceeds the healthy level at which fish live. Over the course of 20 days, C_{BOD} drops significantly. C_{DO} drops over the first 20 days under the circumstances that degradation exceeds reaeration. After the 20 days, reaeration exceeds degradation, causing C_{DO} to gradually return to the healthy level.

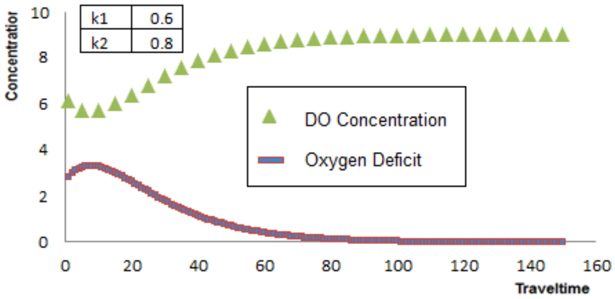

Figure 3. Changes of the DO and oxygen deficit for k_1=0.6 and k_2=0.8

Figure 3 displays the DO curve with k_1=0.6 and k_2=0.8. Over the course of 15 days, C_{DO} drops significantly over the first day under the circumstances that degradation exceeds reaeration. After the 15 days, reaeration exceeds degradation, causing C_{DO} to gradually return to the healthy level.

3. Classifications of Streams

Table 2. Reaeration constants k_r (Source: Peavy, Rowe and Tchobanoglous, 1985)

Water body	**Ranges of k_r** at 20°C,(base e)
Small ponds and backwaters	0.1-0.23
Sluggish streams and large lakes	0.23-0.35
Large streams of low velocity	0.35-0.46
Large streams of normal velocity	0.46-0.69
Swift streams	0.69-1.15
Rapids and waterfalls	Greater than 1.15

Reaeration constant, k_r (O'Connor Equation)

$$k_r = \frac{3.9V^{0.5}\sqrt{(1.037)^{(T-20)}}}{H^{\frac{3}{2}}}$$

V = mean stream velocity (m/sec)
H = average depth of river (m)
T = Temperature in C

4. Nanoparticles to Improve Water Quality

Macro pollutants and micropollutants such as heavy metals and microcystins could not be removed from traditional treatment methods. For the macromolecules and heavy metals, dissolved in water body, to be a valid candidate for chelation with EDTA [8-9], the molecule must be thermodynamically stable (moderately small optimized energy) and have high reactivity (high dipole moment along with multicolored electrostatic map) [6-7]. Figure 4 shows an optimized EDTA molecule and its electrostatic potential map obtained using a computational program.

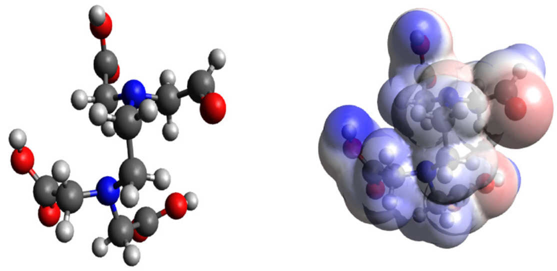

Figure 4. EDTA molecule and its electrostatic potential map

Among the chelates bonded with macromolecules analyzed in this study, magnesium EDTA is the ideal molecule with the lowest optimization representing stability, but Sulfur EDTA has the highest dipole moment representin reactivity. This variation represents that there is a trade off phenomenon for the molecules.

Table 3. Chemical information on the macromolecule EDTA metal chelators

Compounds	**Opt. Energy (kJ/mol)**	**Dipole Moments (Debye)**	**Chemical Formula**	**Molecular Weight (g/mol)**
EDTA (a, control)	188.432	2.541	$C_{10}H_{16}N_2O_8$	292.24
Mg-EDTA (c)	664.237	20.520	$C_{10}H_{12}MgN_2O_8$	312.516
S-EDTA (d)	875.054	30.419	$C_{10}H_{16}N_2O_8S$	320.276
K-EDTA (e)	731.409	20.344	$C_{10}H_{12}KN_2O_8$	327.309
Ca-EDTA (b)	736.047	20.104	$C_{10}H_{12}CaN_2O_8$	328.289

Macromolecules were attached with EDTA chelates then analyzed their optimized energy, dipole moments, and mapped out the optimized shape and electrostatic potential map. Partial chelates analyzed using computational simulations are attached with the macromolecules shown in Table 3.

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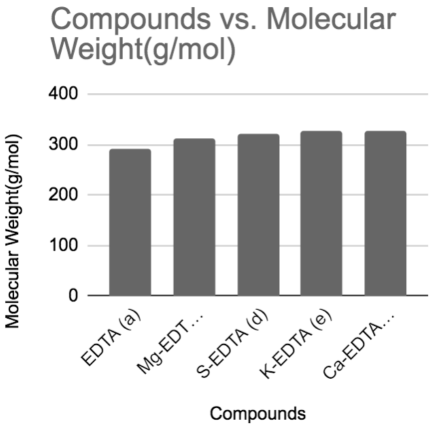

Figure 5. Molecular weights of different metal chelators

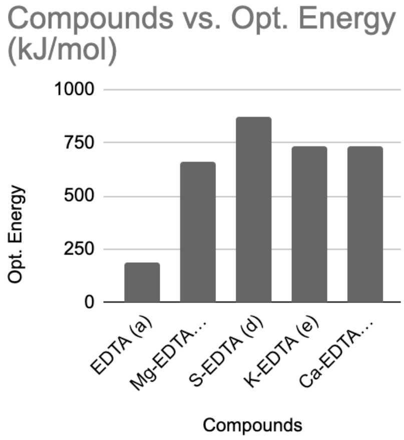

Figure 6. Optimized energy of the different metal chelators

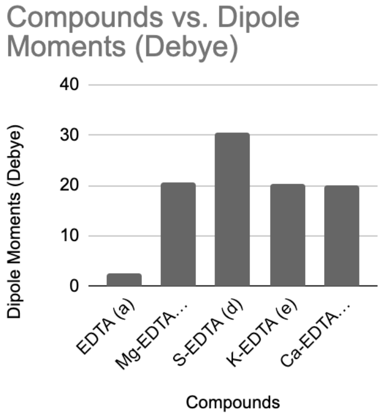

Figure 7. Dipole moments of different metal chelators

Figure 5, 6 and 7 above show the data displaying the optimized energies, dipole moments, and molecular weights of different metal chelators. Again, sulfur EDTA was overall higher in both optimization energy and dipole moments. The optimization energy of magnesium EDTA was overall lowest among other metal chelates, but excluding sulfur EDTA, magnesium had the highest dipole moment among all metals. There seems to be no relationship with the increasing molecular weight and optimization energy and dipole moment.

5. Discussions and Conclusions

Water quality in the water body system undergoes recovery from organic pollution. Even though the initial contraction of DO exceeds a certain level, over the course of time, the contraction of BOD drops significantly. After days, it was found that the reaeration exceeds degradation, causing the contraction of DO to gradually return to the healthy level.

Also we aimed to model several metal chelators through computer software and performed the optimal analysis for such chelators that can be utilized to improve water quality. In this project, various chemical molecules have been studied to be the potential metal ion chelator, where the candidates include a variety of molecules, including EDTA, M-EDTA and other metal-EDTA complexes. These molecules were tested for their thermodynamic stabilities, reactivities, and polarizations, and these characteristics are important factors in selecting the most suitable chelator for metal ion chelation. The three factors such as optimized energies, dipole moments, and electrostatic maps were checked. Stereochemical aspects were also investigated via molecular geometry.

Among the Macromolecules With EDTA chelates, copper EDTA molecules must be thermodynamically stable (moderately low optimization energy), and the chlorine EDTA has a high reactivity (high dipole moment, and saturated electrostatic map). Though in this computational experiment, there seems to be an unusual phenomenon. Boron had the lowest dipole moment compared to other chelators, but had the multi-color electrostatic potential map. This phenomenon can be because of extremely high optimization energy, which means that the molecule is a highly unstable molecule, and thus unlikely that it will exist in nature [6,7].

To summarize, the molecules were assessed for thermodynamic stability, reactivity/conductivity, and polarization. Thermodynamic stability could be measured through the optimized energy, and the smaller the optimized energy, the more thermodynamically stable the molecule was. Reactivity/conductivity was measured through the dipole moments and could speak on the level of activity the molecule could have with another nearby molecule, in this case, plant root.

In this paper, chelates with high dipole moments and low optimized energies are found and they are supposed to be better candidates to keep better water quality.

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