MATHEMATICAL MODELING OF TRANSPORT AND TRANSFORMATION PROCESSES

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ABSTRACT

In this paper we have presented transport and transformation, these process are very important in the study water quality. We discussed advection and diffusion as a transport process and BOD Oxidation and Surface reaeration as a transformation process, which affect all water quality parameters.

Keywords: Diffusion, Transport processes, Turbulent transport'.

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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. 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.

2. STANDARDS AND CRITERIA

Water quality standards are sets of qualitative and quantitative criteria designed to maintain or enhance the quality of receiving waters. Receiving waters are divided into several classes depending on their uses, current or intended, with different sets of criteria designed to protect these uses. For toxic compounds, chemical -specific or whole-effluent approaches can be taken. In the chemical-specific approach, individual criteria are used for each of the toxic chemicals detected in the wastewater. Criteria can be developed in laboratory experiments to protect aquatic life against acute and chronic effects and to safeguard humans against deleterious health effects including cancer [11]. Toxic effects are a function of exposure concentrations as well as their duration. For ex., acute toxicity levels for aquatic life should not be exceeded even for a short time, currently estimated to be on the order of one hour [10]. Chronic toxicity levels can be tolerated for longer times, and a limit currently proposed is based on a four- day average concentration [10]. Human health criteria are typically based on long- term exposures of up to a lifetime so that the corresponding concentration limits are applicable to average values. Allowable frequencies for exceeding the limits may also be specified for the aquatic life criteria, recognizing that it is statistically impossible to ensure that a criterion will ever be exceeded and also that ecological communities are able to recover from stress. The chemical -specific approach, however, does not consider the possible additive, antagonistic, or synergistic effects of multiple chemicals. Nor does it consider the biological availability of the compound, which depends on its form in the wastewater. The whole-effluent approach can be used to overcome the shortcomings of the chemical - specific approach involving the use of toxicity or bioassay tests to determine the concentration at which the wastewater induces acute or chronic toxicity effects. In the whole-effluent

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approach, selected organisms are exposed to effluent diluted in various ratios with samples of receiving water. At various points during the test, the organisms showing various effects, such as lower reproduction rates, reduced growth, or death, are quantified. Toxicity can then be measured in several ways such as the effluent concentration at which 50 percent of the organisms are killed(LC_{50}) or the no observed effect level (NOEL), defined as the highest effluent concentration at which no unacceptable effect will occur even at continuous exposure [10].

3. TRANSPORT PROCESS

The physical, chemical, and biological processes control the fate of the water quality. These processes, are several and varied. It is convenient to divide them into transport processes which affect all water quality parameters and transformation processes, which are constituent -specific. Many of these transformation processes, however, have comparable kinetics so that a different formulation is not required for each constituent.

It is need to reintroduce the conservation of mass equation, which is the basis of practically all further analyses. Here this equation is based on a mass of any water quality constituent in a stationary volume of fixed dimensions, called "control volume.'' The general form of the constituent mass balance can be expressed as follows [1]:

Rate of mass increase in control volume = Rate of mass entering control volume – Rate of mass leaving control volume + Rate of mass generated within control volume – Rate of mass lost within control volume (3.1)

Each of the terms in eq. 3.1 has units of mass per unit time: MT^{-1}. The mass conservation equation is applicable whether the discharge is in a lake, stream, or coastal area. However, the different physical characteristics of these settings require different approaches and approximations to solve for constituent concentrations. In this paper we discussed two basic transport processes advection, or transport of a constituent resulting from the flow of the water in which constituent is dissolved or suspended, and diffusion, or transport due to turbulence in the water.

3.1 Advection:
Using the infinitesimally small, box-like control volume shown in Fig.3-1, the terms of the mass conservation equation relevant to advection in the x direction are [7]
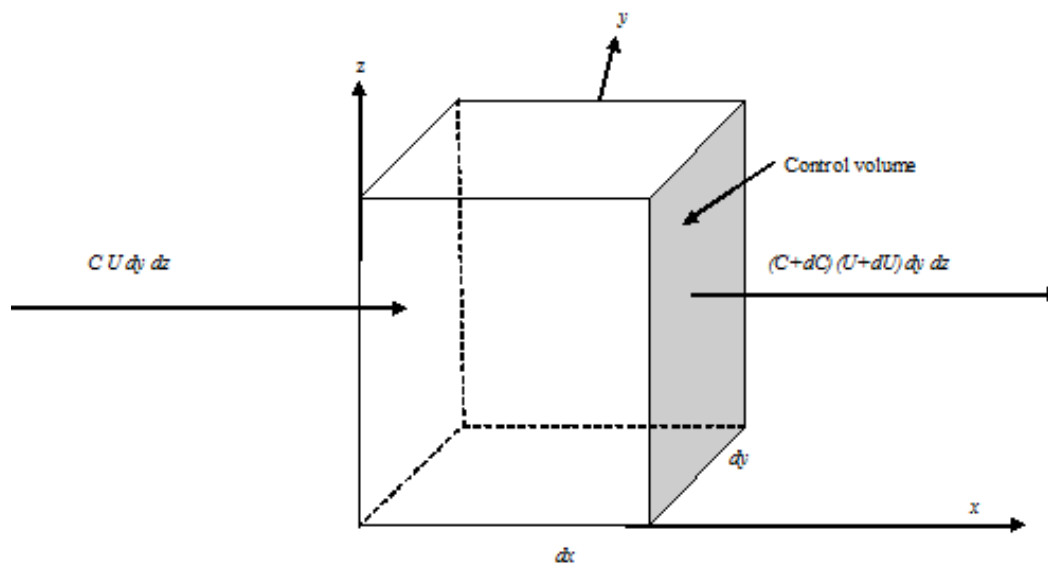

Figure-3.1: Masses of constituent entering and leaving control volume per unit time due to advection in x-direction.

Rate of mass increase in control volume $= \frac{\partial C}{\partial t} dx\, dy\, dz$
Rate of mass entering control volume $= C\, U\, dy\, dz$
Rate of mass leaving control volume $= \left(C + \frac{\partial C}{\partial x} dx \right)\left(U + \frac{\partial U}{\partial x} dx \right) dy\, dz$
Where C = mass concentration of constituent, M/L^3
U= water velocity in x direction, L/T
dx, dy, dz = dimensions of control volume in x, y and z directions, L
t=Time, T
General dimensions rather than specific units are indicated above for the various parameters, as the equations are dimensionally homogeneous. Typically, concentrations are expressed in mg/L, substituting the terms given in Eq. 3.1 and simplifying we get

$$\frac{\partial c}{\partial t} = -U\, \frac{\partial c}{\partial x} - C\frac{\partial U}{\partial x} - \frac{\partial c}{\partial x}\frac{\partial U}{\partial x} dx \qquad (3.1.1)$$

The last term on the right-hand side is negligible compared to the others and can be omitted (because it contains a second -order term).The contributions of flow components in the y and x directions, which are similar to that of flow in the $direction$, must be added in :

$$\frac{\partial c}{\partial t} = -U\frac{\partial c}{\partial x} - C\frac{\partial U}{\partial x} - V\frac{\partial c}{\partial y} - C\frac{\partial V}{\partial y} - W\frac{\partial c}{\partial z} - C\frac{\partial W}{\partial z} \qquad (3.1.2)$$

Where V and W are the velocity components in the y and z directions. A final simplification results when the equation of continuity from fluid mechanics ($\partial U/\partial x + \partial V/\partial y + \partial W/\partial z = 0$) is introduced in Eq.3.1. in the resulting equation, the effect of advection on concentration changes with time is defined [4].

$$\frac{\partial c}{\partial t} = -U\frac{\partial c}{\partial x} - V\frac{\partial c}{\partial y} - W\frac{\partial c}{\partial z} \qquad (3.1.3)$$

3.2 Diffusion:

Turbulent velocity fluctuations in conjunction with concentrations gradients lead to a mass transport phenomenon called "diffusion", which can be described as local mixing by turbulent eddies. The rate of mass transport is proportional to the concentration gradient (or longitudinal rate of concentration variation). Thus, returning to fig. 3.1, the terms of the mass conservation equation relevant to diffusion in the x direction are [5]

Rate of mass increase in control volume $= \frac{\partial c}{\partial t} dx\, dy\, dz$

Rate of mass entering control volume $= -E_x \frac{\partial c}{\partial x} dy\, dz$

Rate of mass leaving control volume $= -\left[E_x \frac{\partial c}{\partial x} + \frac{\partial}{\partial x}\left(E_x \frac{\partial c}{\partial x}\right) dx \right] dy\, dz$

Where E_x = diffusion coefficient (also called diffusivity) in the x direction, L^2/T. Substituting into Eq. 3.1 gives the time rate of change of concentration in the control volume due to diffusion in the x direction:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[E_x \frac{\partial c}{\partial x}\right] \qquad (3.2.1)$$

Adding the equivalent terms for diffusion in y and z directions yields

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left[E_x \frac{\partial c}{\partial x}\right] + \frac{\partial}{\partial y}\left[E_x \frac{\partial c}{\partial y}\right] + \frac{\partial}{\partial z}\left[E_x \frac{\partial c}{\partial z}\right] \qquad (3.2.2)$$

A difficulty with turbulent diffusion is that the corresponding diffusion coefficients are dependent on the flow and thus are non-uniform (variable in space) and anisotropic (direction dependent) [2], [4].

4. TRANSFORMATION PROCESSES

The processes discussed in this section are dependent on the constituent under consideration. For input into the conservation of mass equation, rates of mass gain or loss within the control volume are required. Rates expressions for the major transformation processes are relevant to wastewater discharges.

4.1 BOD Oxidation:

The oxidation of BOD consumes oxygen and thus represents an oxygen sink for the ambient water. Carbonaceous BOD is oxidized first, followed by nitrogenous BOD after about 8 to 12 days. Both carbonaceous and nitrogenous BOD oxidation is first-order processes, with the rate of oxidation (equal to the rate of BOD exertion) proportional to the amount of BOD present [3].

$$r_C = -K_C L_C \text{ and } r_N = -K_N L_N \qquad (4.1.1)$$

Where r_C = rate of carbonaceous BOD loss per unit volume of water, M/TL^3
r_N = Rate of nitrogenous BOD loss per unit volume of water , M/TL^3
L_C = carbonaceous BOD concentration , M/L^3
L_N = Nitrogenous BOD concentration , M/L^3
K_C = rate constant for carbonaceous BOD oxidation, T^{-1}
K_N = rate constant for nitrogenous BOD oxidation, T^{-1}
t = time, T

The constants are often expressed in 1/days. For ambient water quality predictions, the same time unit must be used for these rates as other quantities, such as velocities, and conversion may be required.

For dissolved-oxygen analyses, BOD oxidation represents an oxygen loss, or sink, which occurs at the same rate as the BOD decay, accounting for both carbonaceous and nitrogenous components gives

$$r_0 = r_c + r_N \qquad (4.1.1)$$

where, r_o = rate of oxygen loss per unit time per unit volumeof water due to BOD oxidation , M/TL^3. There are other sources and sinks for dissolved oxygen that need to be considered. These include surface reaeration, sediments oxygen demand, photosynthesis, and respiration but we are discussing only surface reaeration.

4.2 Surface Reaeration:

When the dissolved-oxygen concentration in a body of water with a free surface is below the saturation concentration, a net flux (mass per unit time per unit surface area) is proportional to the amount by which the dissolved oxygen is below saturation for a control volume with a free surface area, the rate of dissolved-oxygen increase due to surface reaeration is therefore [9]

$$r_R = k_R \frac{A}{V}(C_S - C) = \frac{k_R}{H}(C_S - C) = K_2(C_S - C) \tag{4.2.1}$$

Where

r_R = rate of oxygen gain due to reaeration per unit time per unit volume of water , M/TL^3

k_R = reaeration flux rate, L/T

A = free surface area of control volume, L^2

V = volume of control volume, L^3

C_S= Saturation dissolved-oxygen concentration, M/L^3

C= Dissolved-oxygen concentration, M/L^3

H = control volume depth, L

K_2 = Surface reaeration rate, 1/T

We cannot extend the control volume used above down to the bottom of the water body. The control volume must be small enough so that the dissolved-oxygen concentration is approximately uniform. Different control volume depths are thus appropriate for different situations. Therefore, the reaeration rate of greater physical significance is k_R, whereas K_2 depends on the control volume depth. However, for historical reasons, K_2 is used more frequently. a number of empirical and semi-empirical formulae have been proposed to calculate the reaeration rate [6]. Most of these relationships were devised for streams but are frequently applied inn lakes and coastal areas. A commonly used formula is that of O'Conner and Dobbins [8]

$$K_2 = \frac{(D_0 U)^{1/2}}{H^{3/2}} \tag{4.2.2}$$

Where D_0 = molecular diffusion coefficient for oxygen in water, L^2/T;

=18.95 × 10^{-4} ft^2/d (1.76 X 10^{-4} m^2/d) at 20°C, to be multiplied by 1.037^{T-20^oC} for other temperatures, T

U = current speed, L/T

Estimates of K_2 based on the surface renewal model of reaeration see (Eq.4.2.2), are often low b a factor of up to 3, particularly for swift streams [6]. Another approach that can be used to determine K_2 is based on energy dissipation [12]:

$$K_2 = C_e \frac{\Delta h}{t_f} \tag{4.2.3}$$

Where Δh =change in surface elevation, L

t_f = travel time , T

C_e =escape coefficient =0.054 ft^{-1} (0.177m^{-1}) at 20°c, to be adjusted downward for relatively large streams with flow greater than about 250 ft^3/s(7 m^3/s)toward a limiting value of 0.027ft^{-1}(0.09 m^{-1}); for temperatures other than 20^{0}c multiply by $1.022^{(T-20^oC)}$

CONCLUSION

The control volume used above does not necessarily extend down to the bottom of the water body. The control volume must be small enough so that the dissolved-oxygen concentration is approximately uniform. Different control volume depths are thus appropriate for different situations.

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