



## WATER QUALITY ASSESSMENT IN A STOCHASTIC STREAM ENVIRONMENT

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**Abstract:** From a regulatory perspective, the management of stream environments should reflect the uncertainty of the system which they are trying to protect. In light of these factors, methodologies are presented within this article to aid in the quantification of the uncertainty in the management of stream water quality. Specifically, means are developed for: (1) establishing the probability distribution of dissolved oxygen and critical location in a stream; (2) finding the critical location under uncertainty; and (3) quantifying the joint risk of violating a given water quality standard with a known deficit over a specified length of the stream environment.

**Keywords:** dissolved oxygen, biochemical oxygen demand, Monte Carlo simulation, first-order uncertainty analysis, risk assessment, Streeter-Phelps equations, probability distributions.

### Introduction

The physical, biological, and chemical processes occurring within the stream environment are dictated by nature which, in general, cannot be predicted with certainty. To successfully manage the quality of stream environments, techniques should be developed which reflect the uncertainty of the system being managed. From a regulatory perspective, some means within the management process should be developed to account for the concept of risk. Risk, in a water quality sense, defines the probability that a given stream standard will be violated. The risk of violating such standards could be quantified provided the probability distribution of water quality were known.

It is the objective of this article to present methodologies for the assessment of water quality in a stream environment under uncertainty. Means are developed for: (1) establishing the probability distribution of instream DO deficit and location of minimum DO levels (i.e. the "critical location"); (2) finding the critical location in an uncertain stream

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environment; and (3) quantifying the joint risk of violating a known water quality standard with a given DO deficit and length of such violation within a stream environment.

### Basic Water Quality Model

Several mathematical models have been developed to describe the interaction between BOD and DO within a stream. The most well-known mathematical relation of this type is the Streeter-Phelps equation (Streeter-Phelps, 1925). In its basic form, the equation is given as:

$$D(x) = \frac{K_d L_o}{K_a - K_d} \left[ \exp\left(-\frac{K_d x}{u}\right) - \exp\left(-\frac{K_a x}{u}\right) \right] + D_o \exp\left(-\frac{K_a x}{u}\right) \quad (1)$$

where  $K_d$  = the deoxygenation coefficient;  $K_a$  = the reaeration coefficient;  $x$  = the distance downstream from the beginning of each reach;  $u$  = the average stream velocity;  $D(x)$  = DO deficit at a location  $x$ ;  $D_o$  = the initial DO deficit (at  $x=0$ ); and  $L_o$  the initial instream BOD concentration. The location of maximum downstream deficit,  $X_c$ , is found by

$$X_c = \frac{u}{K_a - K_d} \ln \left\{ \left[ \frac{K_a}{K_d} \right] \left[ 1 - \frac{(K_a - K_d) D_o}{K_d L_o} \right] \right\} \quad (2)$$

The point  $X_c$  is herein referred to as the "critical location". The associated maximum DO deficit is determined by

$$D_{\max} = \frac{K_d L_o}{K_a} \exp \left[ -\frac{K_d X_c}{u} \right] \quad (3)$$

### Some Statistical Tools

Before discussing each of the objectives in detail, it is worthwhile to note two statistical tools used throughout this article: (1) Monte Carlo simulation and (2) first-order analysis of uncertainty. An introductory review of each of these techniques is presented below.

Monte Carlo Simulation. - Monte Carlo simulation can be simply described as a sampling method used to approximate, through simulation and the sampling of random numbers, the solution of a non-linear formulation which would otherwise be extremely tedious to solve by direct analytical methods. The foundation for such an application lies in

the large number of trials or iterations that are performed on a proposed model such that a sufficiently large solution set is generated from which a relatively accurate statistical response from a proposed model can be predicted (Kothandaramann, 1968).

**First-Order Analysis of Uncertainty.**- First-order uncertainty analysis provides a methodology for obtaining an estimate of the moments of a function of several (or single) random variables and can be characterized by two vital components: (1) the uncertainty of any parameter or variable is described exclusively by its mean and variance and (2) the series expansion of a functional relationship will contain only the first-order terms (Benjamin and Cornell, 1970). In first-order analysis, a function involving random variables is expanded in a Taylor's series (containing only first-order terms) about the mean values of the model parameters. Then, the expectation and variance operators are applied to the truncated series.

### Joint Risk Assessment

Presently, water quality standards are developed based on a deterministic maximum contaminant level or minimum required concentration, both of which are never to be violated. It seems unreasonable, both environmentally and economically, to continue the enforcement of water quality standards which neglect the uncertain nature of the system the management is attempting to protect. In order to improve the basis for regulatory standards, a probabilistic measure associated with the violation of water quality regulations should be developed. The measure adopted here is the joint probability of simultaneously violating a specified DO concentration and tolerable length of violation (Hathhorn, 1986; Hathhorn and Tung, 1988). The severity of these violations are related to the tolerance level of the stream's biota to a given pollution level and the length of stream (or time) the system is subjected to these conditions. A tradeoff may exist between the allowable level of DO below some standard and the length of stream subject to these conditions. Both maximum and average DO violation conditions are considered (see Figure 1). From this information, water quality management agencies could introduce regulatory measures that limit the maximum probability of violating a minimum DO standard.

**Quantifying the Joint Risk of Violation.**- In reference to Figure 1, the length of violation is defined as the distance within the stream system where the DO profile is below a specified minimum concentration. Using Eq. 1, Newton-Raphson technique is employed to solve the beginning and ending points of violation,  $X_b$  and  $X_e$ . The maximum deficit beyond the

DO standard,  $D'_{\max}$ , is obtained using Eq. 3, while that of an average deficit beyond standard,  $D'_{\text{ave}}$ , is obtained by integrating Eq. 1 over the length of violation and dividing by this same length.

Various pairs of violation conditions, both maximum and average deficits, are generated using Monte Carlo techniques. The risk is calculated by simply computing the ratio of the number of simulation pairs that jointly exceed a specified deficit and length of violation to the total sample size generated. This information can be displayed graphically in a contour map of joint risk (see Figure 2).

### **Probability Distributions for DO Deficit and Critical Location**

Realizing the existence of uncertainties in the modeling of water quality, the prediction of DO deficits or critical locations within a given reach is no longer a deterministic exercise. In assessing such uncertainty, one problem is to quantify the probability distribution functions (PDF) for each (see Figure 3). To do this, first-order uncertainty analysis is used to quantify the moments of the unknown distributions for the DO deficit and critical location. The estimated statistical moments can then be incorporated into a parametric distribution to functionalize each PDF. The question arises, "which probability model best describes the random behavior of the DO deficit or critical location in a stream?" In making such comparisons, one must establish a "true" PDF for each then evaluate the performance of the selected parametric distribution to match or "fit" the true distribution. These steps are briefly outlined in the following subsections. For a detailed discussion of these ideas, the reader is referred to Hathhorn (1986) and Tung and Hathhorn (1988a,b).

**Estimation of the True Distribution for DO Deficit and Critical Location.-** To determine the PDF of the DO deficit and critical location, Monte Carlo techniques are employed using Eqs. 2 and 3. Simulation procedures are performed such that 10 groups of 999 DO deficits or critical locations are generated. Each of the 10 groups of 999 outputs are ranked in ascending order, assigning the minimum value of DO deficit or critical location to the 1-st. position and the maximum value to the 999-th position. The  $p$ -th quantile of DO deficit or critical location is computed by locating the value in position  $(999 + 1)p$ .

**Performance Evaluation of the Selected Distributions.-** Four parametric distributions are considered as potential candidates in representing the PDF of the DO deficits and critical location: normal, log-normal, gamma, and Weibull. To evaluate the relative performance of the four candidate distributions, three criteria are adopted: (1) biasness (BIAS), (2) mean absolute error (MAE) and (3) root mean square error

(RMSE). The distribution which "best fits" is then determined from those selected giving the lowest value for each of the three criteria.

The results of these numerical experiments revealed that, in the majority of cases analyzed, the log-normal and gamma distributions best fit the PDFs for DO deficit and critical location, respectively, regardless of the type of distribution assumed for the model parameters. In addition, it was determined that the 90 percent confidence interval of the critical location was too large to have any practical implication. Nevertheless, knowing the distribution of the critical location may provide useful information in estimating the location of such a point as is discussed in the final section.

### **Finding the Critical Location in a Stream Under Uncertainty**

From a regulatory viewpoint, the critical location is a point which poses the greatest threat to water quality violation. Unlike the deterministic case, the computation of the critical location in a stochastic environment gives rise to uncertainty in its determination. Under uncertainty, the authors suggest a redefinition of the critical location:

- (1) the location determined from Eq. 2 using the mean values of the water quality parameters;
- (2) the location of the maximum variance for the DO deficit;
- (3) the location of maximum probability of violating a given water quality standard;
- (4) the point "most likely" to be critical.

The procedures for quantifying each of these definitions is briefly discussed below. For a detailed presentation and implementation of these ideas, the reader is referred to Hathhorn (1986) and Tung and Hathhorn (1989).

**Location Associated with Mean Valued Water Quality Parameters.-** Essentially, this is a deterministic approach for quantifying the location of the critical point. Mean values for each of the model parameters in Eq. 2 are selected and the equation is solved. Although simplistic in ideology, the utility of such an approach should not be initially overlooked. Results obtained in this manner may be similar to those obtained from more sophisticated techniques.

**Location Associated with the Maximum Variance of DO Deficit.-** Such a point uniquely represents a stream location where the uncertainty in DO prediction is largest. An expression for the variance of DO deficits can be obtained using first-order analysis. From this, the question of finding the location of maximum variance is a problem of unconstrained, non-linear optimization which may be solved by a number of methodologies, for example, Fibonacci search (Beveridge and Schecter, 1970).

Location Associated with the Maximum Probability of Violation.- Unlike any other point in a reach of stream, the point of maximum probability of violation represents a location posing the greatest threat to water quality transgression. It is this location, amongst all others, at which the potential for the destruction of the aquatic biota is most vulnerable. Once the PDF for DO deficit is determined, then the probability of violating a given level of DO at any location may be determined as:

$$\text{Max Pr } (D(x) \geq D_{\text{std}})$$

where  $D_{\text{std}} = D_s - DO_{\text{std}}$  where  $D_s$  and  $DO_{\text{std}}$  are the saturated DO concentration and minimum required DO standard, respectively. Once again, this is a problem of unconstrained, non-linear optimization which may be solved using Fibonacci search.

Location Most Likely to be Critical.- Noting the existence of a PDF for the critical location, the value most likely to occur is commonly known as the mode of the distribution. In reference to the PDF for the critical location (see Fig. 3), the most likely point occurs at the peak of the PDF. If one considers a common parametric distribution for the PDF of the critical location, the mode of such distributions are given in Patel, et al. (1976). Otherwise, the PDF may be functionalized, and the maximum determined using Fibonacci search.

Evaluating the Proposed Methodologies.- Without the ability to verify each of the proposed methodologies, one can make a subjective evaluation of the most appropriate definition. The results of the analysis show widely varying locations for the critical point based on the various definitions. Unless other criteria are developed and evaluated, two definitions are justifiable based on the the number of cases analyzed in this study: (1) the location associated with the maximum probability of violating a water quality standard and (2) the point most likely to be critical. Unfortunately, large uncertainties may arise in determining the PDF for the critical location (see Hathhorn 1986), thus, the location associated with the maximum probability of violating a water quality standard would be the most appropriate.

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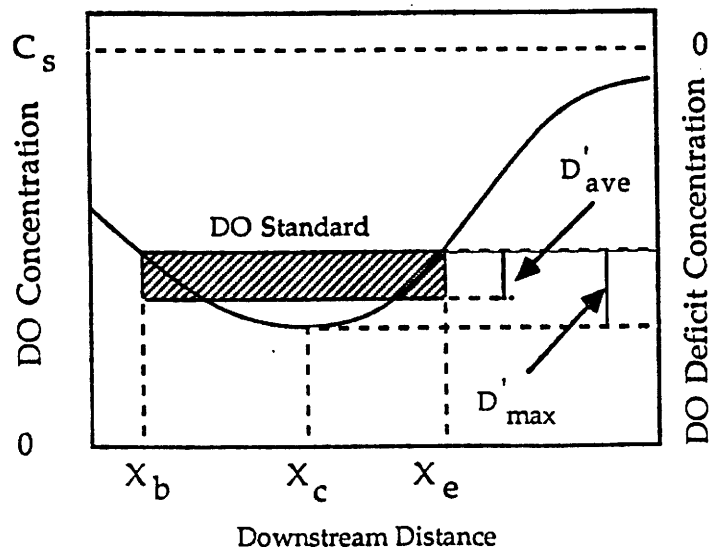


Figure 1. Diagram of Violation Conditions



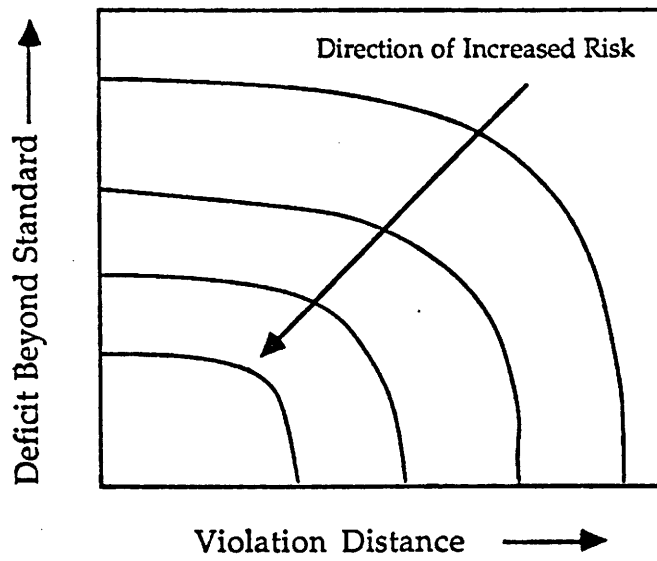


Figure 2. Typical Contours of Joint Risk of Violation

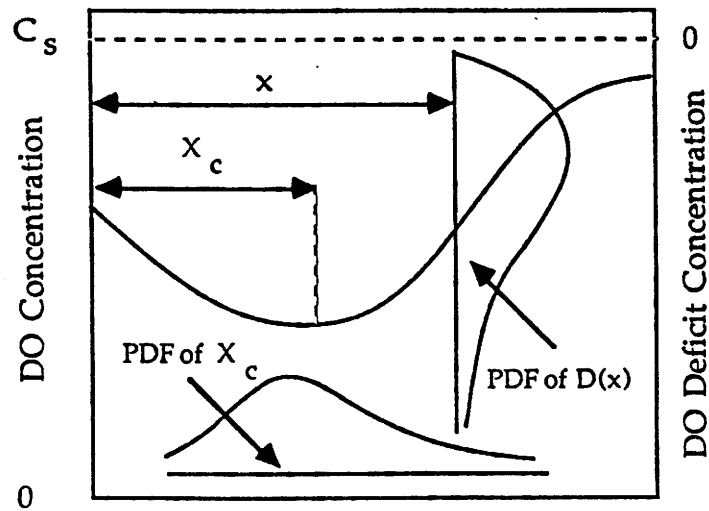


Figure 3. Sketch of PDF for DO Deficit and Critical Location