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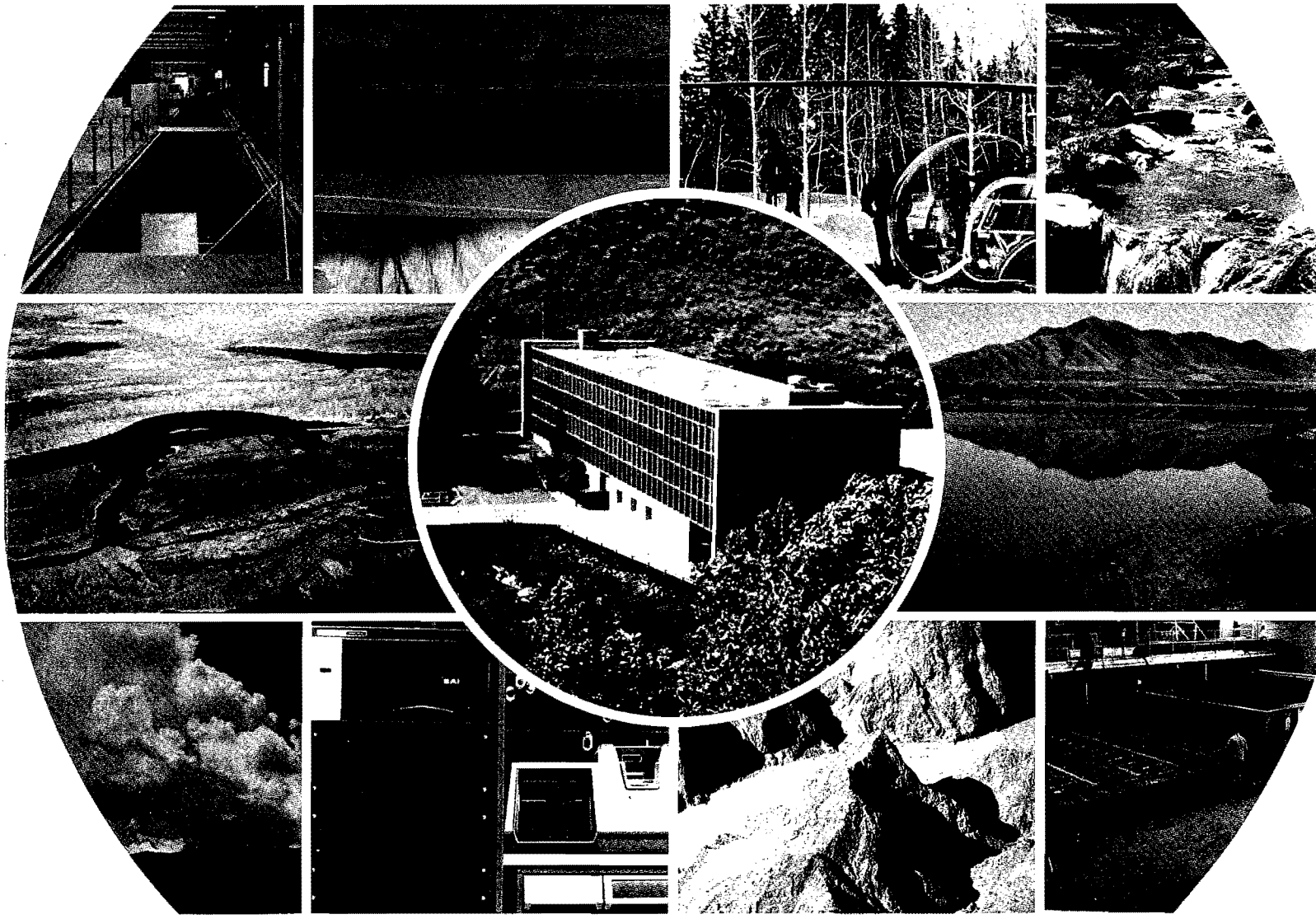

Utah Water Research Laboratory
College of Engineering
Utah State University
Logan, Utah 84322

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WATER QUALITY SERIES
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RANDOM DIFFERENTIAL EQUATIONS IN WATER QUALITY MODELING

by

Brad A. Finney, David S. Bowles, and Michael P. Windham

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ABSTRACT

A probabilistic river water quality model is developed with the capability of determining the joint and marginal probability density function of biochemical oxygen demand (BOD) and dissolved oxygen (DO) at any point in a river. The one dimensional steady-state model can be applied to a river system with any reasonable number of point loads and diversions and lateral surface and subsurface inflow. The model can simultaneously consider randomness in the initial conditions, inputs, and coefficients of the water quality equations. Any empirical or known distribution can be used for the initial condition. The randomness in the water quality equation inputs and coefficients is modeled as a Gaussian white noise process. The joint probability density function (pdf) of BOD and DO is determined by numerically solving the Fokker-Plank equation. Moment equations are developed which allow the mean and variance of the marginal distribution of BOD and DO to be calculated independently of the joint pdf. An upper limit on the coefficient noise variance parameter is presented for which the BOD-DO covariance matrix will be asymptotically stable.

The probabilistic river water quality model is applied to two problems, a sensitivity problem and a hypothetical problem. The sensitivity problem is used to gain familiarity with the simulation model and determine the sensitivity of the model responses to changes in the standard deviation parameter of the input and coefficient noise. The standard deviation parameter of the input noise is varied between zero and 30 percent of the respective input, while the standard deviation parameter of the coefficient noise is varied between zero and 50 percent of the respective coefficient. The model responses are found to be fairly sensitive to changes in the standard deviation parameter of the coefficient noise but relatively insensitive to changes in the standard deviation parameter of the input noise. The possibility of using the moment equations and a normal approximation in lieu of calculating the joint pdf of BOD and DO is discussed. The accuracy of the numerical solution technique for the Fokker-Plank equation is also discussed.

The hypothetical problem is used to evaluate the performance of the model in simulating a more complex river system (which included two point loads) and to evaluate the numerical quadrature algorithm used to determine the joint pdf of BOD and DO immediately downstream of a point load. The numerical solution technique used to determine the joint pdf of BOD and DO remained stable throughout the simulation and the computational costs are judged to be reasonable for a problem of this complexity. The quadrature algorithm was judged to have performed adequately for both the point loads.

ACKNOWLEDGMENTS

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Brad A. Finney
David S. Bowles
Michael P. Windham

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CHAPTER I

INTRODUCTION

Background

In recent years, mathematical water quality models have been developed to simulate the chemical, physical, and biological interactions occurring in river water. These river models have been used to identify important instream processes affecting river water quality, to predict the impact of future development schemes on river water quality, to evaluate alternative pollution control strategies for improving river water quality, and for forecasting water quality for real time control applications. The entire model development and application process is most commonly approached without explicit consideration of the effects of uncertainties on the reliability of model predictions. Model predictions are used as a basis for planning and management studies which lead to costly investments in pollution control which might be significantly altered if the reliability of model predictions were considered.

The practitioner who uses a river model is faced with a task such as the selection of an effective pollution control strategy which will reduce the risk of failing to meet stream or effluent standards to an acceptably low probability. Two types of information are needed before this selection can be made: 1) probability distributions describing the errors in the estimate of the concentrations of water quality constituents obtained from a river model, and 2) data on the economic and other types of consequences resulting from failure to meet stream or effluent standards. By combining these probability distributions and damage functions, optimal strategies, which minimize the expected value of the consequences of errors in model predictions, can be developed. However, few currently available river models have the capability for providing probabilistic output and of those that do only selected types of uncertainties are considered. The work described in this report is the latest in a series of studies performed at the Utah Water Research Laboratory (UWRL) to develop methods for obtaining estimates of the reliability of predictions from river water quality models. The remainder of this background section will be directed to a discussion of the propagation of uncertainties in a river quality model and a brief survey of previous UWRL work which has led up to this study.

Typically river quality models are deterministic in nature in that they provide a single set of model responses for each set of inputs. Blind use of deterministic models implies that there is sufficient information available to be "certain" in making predictions of water quality. In fact, some level of uncertainty is always associated with using a mathematical model to predict the outcome of a natural process. The reasons for uncertainty in model predictions are varied and are represented schematically in Figure 1.1 which is discussed below.

The mathematical structure of the model imperfectly represents the real world physical relationships either because the processes are not completely understood or because a complicated representation is too costly to implement and therefore simplifications must be made. Even if the model structure could be perfect, some uncertainty would result from the inherent variability and randomness in natural processes, most of which can be attributed to the atmosphere as a primary source [*Yevyevich* 1971].

Uncertainty in model structure affects the calibration stage of modeling in which values are assigned to model parameters. Initial parameter estimates based on prior experience or laboratory studies are modified so that the model reproduces measured values reasonably well. Inadequacies in the model structure are, in part, compensated for by adjusting the parameters to maximize some goodness-of-fit criterion within the constraints of the given model structure. Final, or a posterior, parameter estimates are also affected by uncertainty in the measurements which may take the form of unrepresentativeness, measurement errors, or incompleteness. Data may be unrepresentative of simplifying assumptions made at the model building stage, for example, steady-state conditions or completely mixed conditions at each stream cross-section. Measurement errors arise from sampling error, instrumentation noise, analytical error, and data transmission errors. Also data are incomplete in the sense that not all variables are measured, and for those that are measured, the period of data is of finite length and the data are not continuous with respect to either time or space.

Model prediction errors result from several sources: imperfect model structure, parameter estimation errors, numerical solution errors, and uncertainty in initial conditions and model inputs. In addition, estimation theory, and most forecast models, use measurements of the state variables to correct or update model predictions; and therefore, prediction errors are also influenced by uncertainty in these measurements. Initial conditions and inputs are uncertain due to model structure simplifications such as the assumption of steady-state conditions. Also they are uncertain because of uncertainty in estimating future loadings (model inputs) which are based on a water use projection and future waste water technologies.

The first attempt by UWRL to include estimates of prediction reliability in a river water quality model was reported by *Bowles and Grenney* [1978a].

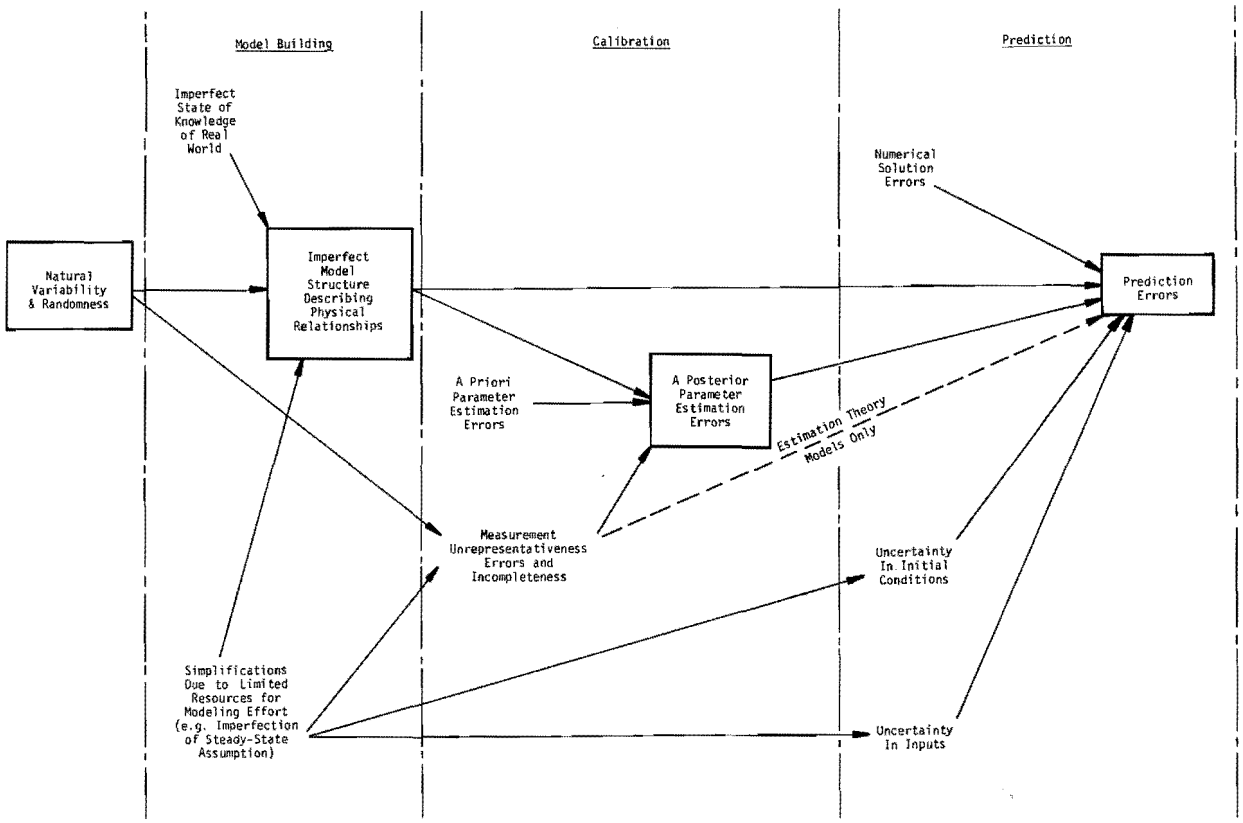


Figure 1.1. Flow of uncertainties in the water quality modeling process.

They used estimation theory in the form of an extended Kalman filter (EKF) which was applied to a steady-state model of BOD-DO and nitrogen cycling in the Jordon River, Utah. The EKF provides a framework for combining measured values of constituent concentrations with model estimates of these concentrations in such a way that approximate minimum variance estimates of the true concentrations are obtained together with the estimation errors representing the reliability of the concentration estimates based on uncertainties in both the measurements and the model structure. A limitation of the EKF is that it always requires measurements on the river system. Thus it is a useful approach for real time forecasting and control but not for prediction of system performance under alternative control strategies for which no measurements on the prototype system are available because to obtain them would require implementing the very control strategies which are under consideration and therefore would remove the advantage of modeling through testing the system response without altering the prototype itself. Other uses of the EKF are model structure identification and model calibration. *Bowles and Grenney* [1978b] used the same EKF model to simultaneously estimate some model parameters. *Bowles and Beck* [1979] have demonstrated the use of two interacting linear Kalman filters for estimating both the water quality concentrations and the model parameters in the River Cam, England. This approach considers uncertainties in the measurements, the model structure, and the model parameters. However, the approach is unsuitable for the prediction problem for the same reasons as stated above for the EKF.

Malone et al. [1979] demonstrated the feasibility of applying several stochastic techniques to linear water quality models. The Monte Carlo, First-Order Analysis, and Generation of Moment Equations techniques were used in a long-term phosphorus model of Lake Washington. Only the effects of uncertainty in the phosphorus loading were examined. *Malone et al.* [1979] also applied the Generation of Moment Equations technique to a conservative steady-state salinity model of the Colorado River system. In this application two types of uncertainty were considered: 1) estimation error associated with the steady-state values of salinity loading, and 2) estimation error associated with salinity loading from irrigated lands. Therefore, both the Lake Washington and Colorado River studies considered only the effects on model responses of the uncertainty in input loading. An additional limitation of the Colorado River study is that it was restricted to conservative substances. However, the work by *Malone et al.* did not require measurements on the prototype system under each condition to be modeled and therefore is suitable for predictive purposes.

The work reported herein is directed to broadening the scope of steady-state probabilistic water quality models suitable for predictive purposes to include uncertainties present in model inputs, parameters, and initial conditions. This involves transforming the differential equations describing the water quality system from deterministic to random or stochastic and provides an

Table 1.1. Comparison of sources of uncertainty treated in UWRL work.

Reference \ Source of Uncertainty	Inputs	Initial Conditions	Parameter Estimates	Model Structure	Measurements
Bowles and Grenney [1978a]		x		x	x
Bowles and Grenney [1978b]		x	x	x	x
Bowles and Beck [1979]		x	x	x	x
Malone et al. [1979]	x				--
Finney et al. [1979]	x	x	x		--

indication of the range over which model predictions are likely to vary due to the types of uncertainties considered. The type of random differential equation used in this work is the Ito equation which is also the basis for the system model in the Kalman filter.

Table 1.1 compares the sources of uncertainty that have been treated in the various UWRL studies. The first three studies [*Bowles and Grenney* 1978a, b, and *Bowles and Beck* 1979] utilize estimation theory and are suitable for model identification, model calibration, and real time applications for which measurements on at least some of the state variables are available. The current work and that by *Malone et al.* [1979] are suitable for off-line predictive applications for which measurements on the state variables are not available.

Objective

The overall objective of this study is to attempt application of random differential equations to river water quality modeling and to evaluate the results. To achieve this objective, a model is developed to represent two water quality constituents, biochemical oxygen demand (BOD) and dissolved oxygen (DO). A system of random differential equations is used to simulate river water quality in the spatial dimension (*i.e.*, under steady-state conditions). The equations allow the simultaneous consideration of random initial conditions, random inputs, and random model coefficients. The joint probability density of the two quality constituents is determined. The model is applied to a river system for testing and evaluation. The sensitivity of the joint probability density to input and coefficient randomness is investigated.

Summary of Contents

A review of river water quality models in which the state variables (quality constituents) are treated as random variables is presented in Chapter II. The models are classified by the manner in which the randomness is represented and the techniques used to determine the distributional properties of the state variables.

A detailed description of the probabilistic water quality simulation model developed as part of this study is presented in Chapter III. Sections on river system layout, program procedure, water balance equation, and water quality equations are included. The numerical aspects of the model are also described.

Application of the probabilistic river water quality model is described in Chapter IV. To gain familiarity with the model, it is first applied to a sensitivity problem. The sensitivity of the model responses to several input parameters is investigated. The results of the model application to a hypothetical river system are then presented. A section on computational requirements of the model is also included.

A summary of the research accomplished in this study is contained in Chapter V. In addition, several conclusions and recommendations for further work are made.

Data input formats, a program listing for the probabilistic river water quality model (PSSAM), and an example computer printout of the model application are available at a nominal charge by writing to: The Librarian, Utah Water Research Laboratory, College of Engineering, Utah State University, UMC 82, Logan, Utah 84322.

CHAPTER II

LITERATURE REVIEW

According to *Morse* [1978], mathematical modeling of physical systems is in transition from a deterministic toward a nondeterministic (random) philosophy. He concluded that this trend was the result of the scarcity and cost of real-world data, skepticism over the data which are available, and attempts by researchers to introduce more natural formulations to physical and biological sciences problems. While most of the water quality models currently in use are deterministic (for example, Qual II, *Environmental Dynamics, Inc.* [1971]; SSAM, *Grenney and Porcella* [1975]; *Bowles et al.* [1975]; and *HEC* [1979]), a number of models have been proposed in recent years which treat the water quality constituents as random variables. The main differences in these models are the types of randomness which are treated, and the solution process used to solve the resulting random equations.

Probabilistic Water Quality Models

The following discussion covers all types of probabilistic water quality models except those that use Ito differential equations. The models using Ito differential equations will be discussed in the next section.

Loucks and Lynn [1966] proposed a model that predicts the probability density of biochemical oxygen demand (BOD) and dissolved oxygen (DO) in a stream with time varying flow. *Loucks and Lynn* modeled the daily streamflow using a discrete first order Markov chain. In the most flexible of their four models, the daily flow from a point load (source of BOD) was correlated with the daily streamflow and the previous day's flow. A conditional probability distribution for BOD was associated with each stream and point load flow. The concentrations of BOD in the stream and point load were assumed to be independent of each other.

Thayer and Krutchkoff [1967] developed a random model for BOD and DO in unsegmented streams. The *Thayer and Krutchkoff* model was a discrete time model. The BOD and DO concentrations were also discretized, with the time Δ introduced to represent the optimum unit size. A change of size Δ constituted a change of one "state." By assuming that the probability of a change of state followed a birth-death process, *Thayer and Krutchkoff* were able to derive the probability distribution of BOD and DO at any point downstream of a point load provided the process coefficients and initial conditions were assumed constant.

Moushegain and Krutchkoff [1969] extended the *Thayer and Krutchkoff* model to permit segmentation of the stream. They assumed that probability output from one segment could be used as the initial condition for the next segment. Although this was a crude approximation which neglected the effect of the spatial probability distribution of BOD and DO, *Moushegain and Krutchkoff* reported it worked quite well.

Custer and Krutchkoff [1969] extended the *Thayer and Krutchkoff* model to estuaries. The random nature of diffusion in an estuary was represented by a random walk process. This model was later modified by *Stochastics Incorporated* [1971] to include random diffuse loading.

Mehta et al. [1975] used Autoregressive Integrated Moving Average (ARIMA) models to describe the random nature of a water quality time series. The time series included daily measurements of streamflow, water temperature, BOD, and DO. With the exception of BOD, the ARIMA models provided satisfactory results. Although *Mehta et al.* did not generate the probability distribution of the stream parameters (flow and temperature) and quality constituents (BOD and DO), they could have done so by Monte Carlo simulation.

Monte Carlo simulation can be thought of as "synthetic sampling." Repeated application of a deterministic simulation model using initial conditions, inputs, and coefficients randomly selected from their probability distribution are used to produce an ensemble of synthetic time series which can then be analyzed to define the statistical characteristics of the system response.

A number of researchers have used Monte Carlo simulation in water quality modeling. *Brutsaert* [1975] determined the cumulative probability density function of the location and the numerical value of the maximum dissolved oxygen deficit (DOD) for a hypothetical stream using Monte Carlo sampling. Initial conditions, flow, and BOD and DO reaction rate coefficients were assumed to be triangularly distributed random variables.

Kothandaraman and Ewing [1969] performed a study similar to *Brutseart*'s although they only considered randomness in the BOD and DO reaction rate coefficients. Using data from the Ohio River, *Kothandaraman and Ewing* determined that the BOD first-order decay rate and the reaeration rate had a distribution that was approximately normal. Assuming that these reaction rate coefficients were indeed normally distributed, a DOD profile of the Ohio River was obtained for 200 synthetic samples using Monte Carlo simulation. The most probable value (mode) of the resulting distribution of DOD compared favorably with the measured data.

In a similar study, *Esen and Bennet* [1971] also used Monte Carlo simulation to determine the DOD distribution in a stream. The BOD first-order decay rate and the DO reaeration rate coefficients were modeled with a random walk process. The model had

the advantage of considering the changes in the mean and variances of these coefficients with travel time.

Shih [1975] investigated the use of Monte Carlo simulation for regional water quality control. A water quality model which allowed random stream flow and random point load flow and effluent concentration was linked with a chance-constrained quadratic programming optimization model. The optimization model determined maximum allowable point load effluent levels subject to the DO standard being maintained in the river.

Whitehead and Young [1979] applied Monte Carlo simulation to a dynamic, stochastic model of river water quality. Using a daily timestep, with random stream flows, point load flow and effluent quality, and reaction rate coefficients, BOD and DO profiles for 185 summer seasons were generated. The observed and forecast BOD and DO cumulative probability distributions showed excellent agreement.

Two major issues must be resolved when the Monte Carlo simulation technique is used: 1) generation of random numbers from a desired distribution, and 2) estimation of the required sample size. *Malone et al.* [1979] concluded that although the Monte Carlo technique is flexible and conceptually simple, it often requires a great deal of computer time to generate the sample size required to assure reasonably accurate estimates of the probability density function of the system's response.

DiToro and O'Connor [1969] considered the effects of two types of time variable flow on the BOD and DO probability distributions in a stream. The first type of variable flow considered had an arbitrary but known (deterministic) time variation. By introducing the concept of release time, the time $\tau(x,t)$ at which the slug of water being observed at point x at time t had previously been released at point $x = 0$, the classical Streeter Phelps BOD-DO equations could be solved for time varying flow. *DiToro and O'Connor* then considered streamflow to be composed of a deterministic and a random component. By assuming a Gaussian normal distribution with zero mean for the random component of flow, they were able to solve for the mean and variance of the BOD and DO concentrations using first-order uncertainty analysis.

The two major components of first-order analysis are: 1) first-order approximation of the functional relationship between variables, and 2) definition of the random component of a variable solely by its variance [*Cornell* 1972]. First-order uncertainty analysis only provides estimates of the mean of the random state variable and variance for nonlinear functional relationships which, with the exception of the normal distribution, do not define the entire probability distribution. Furthermore, *Burgess and Lettenmaier* [1975] state that the analysis is only approximately correct if the variance is small compared to the mean. For linear functional relationships, the mean and variance determined by first-order analysis are exact. Researchers who have used first-order uncertainty analysis in water quality models include *Thomann* [1967], *Chamberlain et al.* [1974], and *Burges and Lettenmaier* [1975].

Chamberlain et al. and *Burges and Lettenmaier* proposed models to estimate the mean and standard deviation of BOD and DO resulting from a single point load in streams where the initial concentration of BOD and DO and the stream velocity were assumed to be normally distributed random variables. *Burges and Lettenmaier* also considered the reaction rate coefficients to be normally distributed random variables. A Monte Carlo simulation used for comparison purposes showed nearly identical results as those from the first-order analysis model near the point load. The BOD and DO probability distributions determined by their first-order analysis model, however, were shown to be increasing as the distance from the point load increased. *Burges and Lettenmaier* determined that the skew in the distributions of both BOD and DO, which increased as a function of distance downstream of the point load, was responsible for the error.

Another method for determining the mean and variance of a water quality parameter was explored by *Morse* [1978]. Using a random forcing function (input) and random initial conditions, a deterministic stream temperature equation was recast as a random nonlinear Voltera integral equation. *Morse* claimed that this model offers the possibility of a temperature forecast more "honest" than deterministic models can provide because it predicts a temperature distribution instead of a single value.

In a series of articles by *Padgett* [1975], *Padgett and Durham* [1976], and *Padgett et al.* [1977], a stochastic model for BOD and DO in streams is presented. The model assumes that the initial condition and point and diffuse load inputs of BOD and DO are random variables. The model is unique in that the joint and marginal probability density functions of BOD and DO can be determined at any location in the stream for any assumed distribution (gamma, binomial, normal, etc.) of the random variables.

Probabilistic Water Quality Models Using Ito Differential Equations

First-order differential equations have been found to give an adequate representation of water quality in many river studies. A special class of random differential equations which has found application in water quality modeling is the Ito differential equation. This is a first-order random differential equation in which the rate of change with respect to time of the vector of water quality concentrations, $\underline{X}(t)$, is a function of a deterministic component and a random component comprising Gaussian white noise processes. The Ito differential equation has the form:

$$\dot{\underline{X}}(t) = \underline{f}(\underline{X}(t), t) + G(\underline{X}(t), t)\underline{W}(t), \quad t \in T$$
$$\underline{X}(t_0) = \underline{X}_0 \tag{2.1}$$

where $\underline{X}(t)$ is an n-dimensional vector of water quality constituent concentrations treated as random variables, $\underline{f}(\underline{X}(t), t)$ is an n-dimensional deterministic vector function, $\underline{W}(t)$ is an m-dimensional vector random process whose components are white noise, $G(\underline{X}(t), t)$ is an $n \times m$ matrix function, and $\underline{X}_0$ is independent of $\underline{W}(t)$, $t \in T$.

Jazwinski [1970] defines a white noise process $\{\underline{W}_t, t \in T\}$ as a Markov process for which

$$P(\underline{W}_t|\underline{W}_\tau) = P(\underline{W}_t),\ t > \tau \in T \qquad (2.2)$$

(Read the probability of W_t given W_τ equals the probability of W_t). That is, the W_t's are mutually independent at all $t \in T$. As a result, knowing the realization of W_τ in no way helps in predicting what W_t will be. A white noise process is completely random or totally unpredictable. If the W_t's are normally distributed for each $t \in T$, then the process is a white Gaussian noise process. Because the process is Gaussian, its probability density is specified by the mean value vector

$$E[\underline{W}_t] = \underline{0} \qquad (2.3)$$

and the covariance matrix

$$E[(\underline{W}_t - E[\underline{W}_t])(\underline{W}_\tau - E[\underline{W}_\tau])^t] = Q(t)\delta(t - \tau) \qquad (2.4)$$

where $Q(t)$ is the covariance matrix of W and $\delta(t - \tau)$ is the Dirac delta function (unity at $t = \tau$, zero otherwise).

Unfortunately, the white noise process is about the "worst behaved" process imaginable [*Schweppe* 1973]. For fixed t, it is a zero mean random vector with an infinite covariance matrix. It is not continuous anywhere and it does not exist in any physical sense. White noise process models are used because powerful techniques exist for obtaining the solution of the process generated by Equation 2.1. In many situations their use can be justified because their effects are approximately the same as those of physical processes when they pass through the same system. *Schweppe* [1973] argues that although a white noise process is only an approximation, all mathematical models are really only approximate representations of the real world.

Bowles et al. [1977], *Koivo et al.* [1976], and *Moore et al.* [1976] used Gaussian white noise processes in applying estimation theory to water quality modeling. All three models considered propagation of prediction uncertainty due to initial condition, model and measurement uncertainty, each represented by Gaussian white noise processes. *Bowles et al.* and *Koivo et al.* estimated not only the state of the systems (*i.e.*, means and variance of the water quality variables), but also demonstrated the usefulness of estimation theory in providing estimates of uncertain process model coefficients. *Moore et al.* demonstrated the sampling design capabilities of estimation theory.

Harris [1976] and *Harris* [1977] applied a first-order Monte Carlo simulation algorithm for multivariable nonlinear stochastic integral equations to determine the mean and variance of BOD and DO in a stream. The algorithm assumes that the uncertainty in flow rate and point load inputs to the system are Gaussian white noise processes. *Harris* compared the results from 5,000 simulated sequences of a four state stochastic differential system with theoretically known results and found that the sample means and covariances were indistinguishable. It appears that *Harris'* algorithm requires the same amount of computational effort as a simple Monte Carlo simulation.

Malone et al. [1979] demonstrated that two techniques, first-order analysis and generation of moments equations, provide exact estimates of the means and covariances for systems of linear Ito differential equations (white noise inputs only) at a fraction of the computational effort required for Monte Carlo simulation. The generation of moments technique, which allows direct calculation of the distributional moments of the state variables, was preferred over the first-order analysis by *Malone et al.*, because the functional relationships between variables must be differentiable to use first-order analysis, not a requirement with the generation of moments technique. The discrete time formulation of the generation of moments technique used by *Malone et al.* in modeling the cycling of phosphorus in Lake Washington was also used by *Morse et al.* [1976].

There is little disagreement that the initial conditions, inputs, and reaction rate coefficients of the aquatic processes are random variables. There appears, however, to be some question as to relative importance of the randomness in the reaction rate coefficients in the resulting probability density function of the state variables. *Whitehead and Young* [1979] found BOD and DO predictions insensitive to coefficient variability provided the variability was within the error bounds defined by an estimation algorithm. *Kothandaraman and Ewing* [1969] and *Burges and Lettenmaier* [1975] found the probability distribution of BOD and DO to be very sensitive to uncertainty in the first-order BOD decay rate and the DO reaeration rate coefficients. *Yu* [1972] found the cost of upgrading sewage treatment plants discharging to a river necessary to meet instream DO standards to be extremely sensitive to the DO reaeration rate.

Most probabilistic water quality models do not have the capability to consider the reaction rate coefficients as random variables. The difficulty in obtaining solutions to differential equations with random coefficients as noted by *Padgett* [1975] and *Soong* [1973] is undoubtedly the primary reason for many models considering the reaction rate coefficients to be deterministic.

Some probabilistic river water quality models using Monte Carlo simulation and first-order analysis and reviewed above have the capability of simultaneously considering random initial conditions, inputs, and reaction rate coefficients, but both techniques have severe limitations. Monte Carlo simulation may be cost prohibitive if the number of samples required to adequately describe the probability distribution of the state variables is too large. The number of samples required increases with the variance and skew of the initial distribution [*Wallis et al.* 1974]. *Wallis et al.* found that for a coefficient of skew greater than five, 100,000 samples were inadequate to satisfactorily describe the tails of the distribution above the 99.9 percent probability level. *Burges and Lettenmaier* [1975] show that first-order analysis, which only predicts the mean and variance of a distribution, was inadequate for a coefficient of skew equal to -1.4.

In summary, although the initial conditions, inputs, and reaction rate coefficients of aquatic

processes are random variables, most probabilistic water quality models do not have the capability to consider them as such. The model developed in this study and described in the next chapter can simultaneously consider all three to be random variables and yet does not have the limitations of Monte Carlo simulation and first-order analysis.

CHAPTER III

DESCRIPTION OF PROBABILISTIC RIVER WATER QUALITY MODEL

Introduction

In Chapter II it was noted that to adequately represent the uncertainty in the prediction of river water quality, it is often necessary to consider simultaneously the randomness in the initial conditions, inputs, and reaction rate coefficients. In this chapter a water quality model that has those capabilities is described.

Although many deterministic water quality models in use are dynamic models, a steady-state model was used in this study with the independent variable being travel time, which is a surrogate for distance along the river. The reasons for using a steady-state model are: 1) in many stream assessment studies the steady-state assumption yields answers to management questions that are of an appropriate resolution, and that are consistent with data availability determined by fiscal and time constraints, 2) lack of available data to calibrate a dynamic model, and 3) the higher computer costs associated with a dynamic model [*Bowles et al.* 1977]. The steady-state model developed in this study, Probabilistic Stream Simulation and Assessment Model (PSSAM), can be applied to a river system with diffuse surface inflow, groundwater inflow (or outflow), and any reasonable number of point loads and point diversions. The deterministic water quality equations in PSSAM were patterned after the Stream Simulation and Assessment Model (SSAM) developed by *Grenney and Porcella* [1975].

This chapter contains the development and solution of the river water quality model in random differential equation form. After introductory sections on the method for describing the layout of a river system and the general operation of the computer model, the deterministic equations for flow balance and water quality are derived. The deterministic water quality equations are then cast in the form of an Ito random differential equation with uncertainty in the initial conditions, input variables, and model coefficients (parameters). Solutions for the joint pdf of BOD and DO are given for control volumes in a section of river with and without point loads or tributaries. Approximate solutions based on moment equations are also given. The chapter closes with sections describing the numerical solution techniques used to obtain the pdf's and a summary of the model limitations.

River System Layout

Seven types of calculation points are used in PSSAM to describe a river system. These seven point types are described below:

HEADWATER (H) -- An upstream boundary of a section which marks the beginning of the first reach.
REACH (R) -- The upstream boundary of a section of river channel having uniform physiochemical characteristics.
POINT LOAD (L) -- Location of a point load discharging into the river.
POINT DIVERSION (D) -- Location of a point diversion from the river.
CHECK POINT (C) -- An additional point along the river where calculated output is desired.
EVAPORATION (E) -- The upstream boundary of a reach where evaporation is significant (*i.e.*, a lake, reservoir, swamp area, or reach with phreatophytic vegetation).
TERMINAL POINT (T) -- The most downstream point in the river system which is modeled.

Figure 3.1 shows a river system having a headwater, seven reaches, two point loads, two point diversions, and three check points. Lateral inflow rates from surface water (Q_S) and groundwater (Q_G) are shown along reach number four.

All model calculations are conducted in metric units. A user option is available to allow English units to be used for input or output.

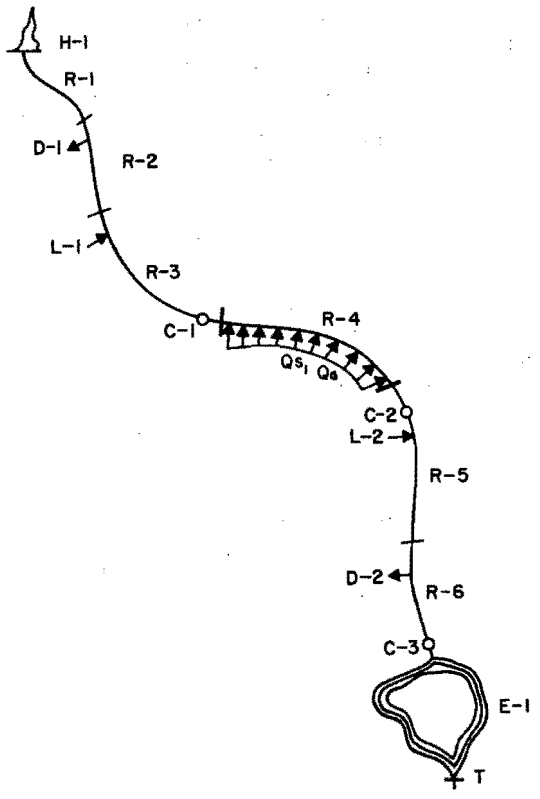


Figure 3.1. Example of a river system layout for PSSAM (notation explained in text).

Program Procedure

The program examines the system layout input data and assigns a sequence number (numbered in sequence from the headwater) to each calculation point in the input. A user option is available to have the program automatically assign additional calculation points at specified intervals within reaches. The segment of channel between two calculation points is defined as an "element." An element is a subsection of a reach. The calculations made by the model start at the headwater and proceed downstream considering each calculation point in sequence. Changes in flow and water quality which occur during passage through an element are modeled by a system of differential equations to be described below. Conditions resulting at the end of one element are used to calculate the boundary conditions at the beginning of the next downstream element.

Program calculations incorporate three distinct steps: 1) simulation of the river flows, 2) description of the point and diffuse loadings on the system by the water quality constituents to be modeled, and 3) simulation of the concentrations of the water quality constituents at each calculation point. A user option is available to stop the program at the end of any step as desired.

The differential equations for step 1 are solved independently from the differential equations representing the water quality constituents (steps 2 and 3). Step 1 starts with the headwater flow and proceeds downstream conducting a flow balance by adding (or subtracting as appropriate) lateral surface flow, lateral subsurface flow, point load flows, and diversion flows. In addition to calculating flows, the model determines the average velocity, cross-sectional area, and hydraulic radius of each element. A summary of the system layout, flow, and stream characteristics is printed out to facilitate checking the input flow data and to provide a concise display of the important features of the river system.

The second step in the model is reading the appropriate data for the water quality constituents. A summary of the water quality data and the coefficients (after temperature adjustment, if appropriate) is printed out to facilitate checking the input water quality data and to provide a concise display of the constituent loadings on the system.

The third step in the program is the prediction of constituent concentration joint and marginal probability distributions along the river for the specified flow and loading patterns. Basically, the model simulates the reactions and interactions among constituents occurring in a control volume (*C.V.*) of water as it travels downstream at a velocity $\bar{V}$. It is assumed that mixing with adjacent *C.V.*'s (dispersion) is negligible. Mass can be added to the *C.V.* by lateral inflow and by leaching from the bottom. Oxygen can enter the *C.V.* by diffusion across the air-water interface and by the photosynthetic oxygen production of benthic and planktonic algae. These reactions and mass transport phenomena are represented in the model by a system of differential equations.

In the prediction step, as in the case of the flow balance step, the model starts at the headwater, where the joint probability density function of the water quality constituents is known. This probability density function provides the initial conditions for the system of equations. Then the joint probability density function, which results from what occurs in the *C.V.* before it reaches the next downstream calculation point, is estimated. A mass balance is conducted on the *C.V.* at this point to account for mass added by point loads, and the resulting concentration probability distribution becomes a new initial condition for the next downstream *C.V.* Then the equations are solved to estimate the concentrations which will occur in the *C.V.* by the time the flow reaches the next downstream calculation point. The model proceeds downstream, element by element, in this manner.

Flow Balance Equations

Flow is assumed to be steady (invariant with time at each calculation point) for the entire system. Surface and subsurface lateral inflow is assumed to be constant per unit distance along the stream whereas subsurface lateral outflow is assumed to be a constant fraction of the flow in the stream. Therefore, when the lateral subsurface flow is positive (*i.e.*, flows into the main stream), the flow downstream of an element can be represented by the following equation:

$$\frac{dQ}{d\tau} = Q_S\bar{V} + Q_G\bar{V} \qquad (3.1)$$

in which

Q = main stream flow (m^3/sec)

τ = travel time (sec)

$\bar{V}$ = average velocity in the main stream (m/sec)

Q_S = lateral surface flow (m^3/sec/m)

Q_G = lateral subsurface flow (m^3/sec/m)

Equation 3.1 represents the change with travel time of the streamflow rate. Travel time is used as the independent variable rather than distance along the channel so that water quality reaction rates can be expressed in terms of day^{-1} rather than m^{-1}. The first term on the right hand side of Equation 3.1 is the rate of change of flow due to surface lateral inflow and the second term represents the rate of change of flow due to subsurface lateral inflow. The solution to Equation 3.1 is:

$$Q = Q_0 + (Q_S + Q_G)\,\Delta x \qquad (3.2)$$

and

$$\Delta x = \bar{V}\Delta\tau \qquad (3.3)$$

in which

Q_0 = flow at the start of the element (m^3/sec)

Q = flow at the end of the element (m^3/sec)

Δx = length of the element (m)

$\Delta\tau$ = travel time through the element (sec)

The average flow ($\bar{Q}$) in the element is:

$$\bar{Q} = \frac{Q + Q_0}{2} \qquad (3.4)$$

When the stream is recharging the groundwater (*i.e.*, lateral subsurface flow is negative), it is assumed that the recharge rate varies with the flow in the stream so that the flow in an element can be represented by the following equation:

$$\frac{dQ}{d\tau} = Q_S\bar{V} - K_G\bar{V}Q \qquad (3.5)$$

in which

K_G = the fraction of main stream flow lost per meter.

Using Equation 3.3, the solution to Equation 3.5 is:

$$Q = \frac{Q_S}{K_G} + \left(Q_0 - \frac{Q_S}{K_G}\right)e^{-K_G\Delta x} \qquad (3.6)$$

It can be shown that the average flow in the element is:

$$\bar{Q} = \left[\frac{Q_S}{\Delta x K_G^2} - \frac{Q_0}{\Delta x K_G}\right]\left[e^{-K_G\Delta x} - 1.0\right] + \frac{Q_L}{K_G} \qquad (3.7)$$

The average velocity ($\bar{V}$) in an element is calculated by the equation:

$$\bar{V} = \beta_1\bar{Q}^{\beta_2} \qquad (3.8)$$

in which

β_1 and β_2 = empirical coefficients for a stream reach

Two options are available to the user for calculating the average hydraulic radius ($\bar{R}$) of an element which is used in the water quality equations. One option is based on Manning's equation expressed as follows:

$$\bar{R} = \left[\frac{n\bar{V}}{\bar{S}^{1/2}}\right]^{1.5} \qquad (3.9)$$

in which

$\bar{S}$ = average hydraulic gradient of a stream reach

n = Manning's coefficient for the reach

The other option is based on an empirical relationship between the hydraulic radius and the average cross-sectional area of the flow ($\bar{A}$):

$$\bar{R} = \beta_3\bar{A}^{\beta_4} \qquad (3.10)$$

and

$$\bar{A} = \frac{\bar{Q}}{\bar{V}} \qquad (3.11)$$

in which

β_3 and β_4 = empirical coefficients for a stream reach

Deterministic Water Quality Equations

General equation

The water quality equations used in PSSAM were patterned after deterministic equations in *Grenney and Porcella* [1975]. In this section the theory of the deterministic equations will be explained. In the next section these deterministic equations will be recast as random equations.

In their final form the water quality equations used in PSSAM measure steady-state conditions but their derivation commences with the one-dimensional channel transport equation (unsteady, nonuniform flow) and follows the steps necessary to represent steady-state conditions and uniform flow:

$$\frac{\partial(AX)}{\partial t} = \frac{\partial}{\partial x}\left(AD\frac{\partial X}{\partial x}\right) - \frac{\partial(VAX)}{\partial x} + SA \qquad (3.12)$$

in which

X = constituent concentration (mg/ℓ)

t = time (sec)

x = distance along the channel (m)

A = cross-sectional area (m^2)

D = longitudinal dispersion coefficient (m^2/sec)

V = average velocity over the cross-section (m/sec)

S = other sources and sinks (mg/ℓ/sec)

Equation 3.12 represents the rate of change with time of the mass of the constituent being transported through some control volume (Figure 3.2). It should be noted that in Equation 3.12 the independent variables are real time (t) and distance along the channel (x). The final water quality equations will be a function of travel time (τ) as are the flow balance equations. The first term on the right-hand side of the equation represents the downstream transport of the material associated with the dispersion due to nonuniform velocity gradients in the river profile. The second term represents the downstream advection of the material and the third term represents the addition or removal of the constituent by lateral inflow (diffuse) benthic loading.

If the longitudinal dispersion is assumed negligible, the flow is assumed nonuniform (inflow allowed), sources and sinks are assumed to be from the lateral surface and subsurface flow and the streambed, and Q is substituted for VA, Equation 3.12 becomes:

$$\frac{\partial(AX)}{\partial t} = X\frac{\partial Q}{\partial x} - Q\frac{\partial X}{\partial x} + Q_S X_S + Q_G X_G + \frac{LA}{R} \qquad (3.13)$$

in which

Q = river flow (m^3/sec)

Q_S = lateral surface inflow (m^3/sec/m)

Q_G = lateral subsurface inflow (m^3/sec/m)

L = benthic leaching rate (mg/m^2/sec)

R = hydraulic radius (m)

X_S = constituent concentration in lateral surface inflow (mg/ℓ)

X_G = constituent concentration in lateral subsurface inflow (mg/ℓ)

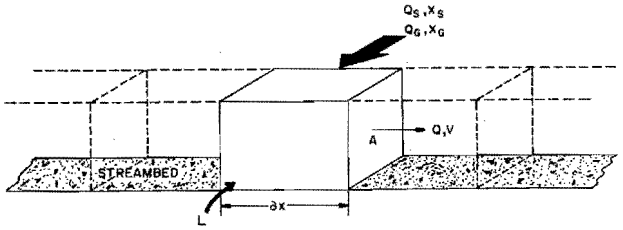


Figure 3.2 Model conceptualization of a stream control volume.

Note that by neglecting dispersion, Equation 3.12 is greatly simplified but that this imposes a limitation of the model's capability to simulate water quality parameters in streams where dispersion is significant.

If steady-state is assumed:

$$\frac{\partial(AX)}{\partial t} = 0$$

Equation 3.13 can be simplified to:

$$\frac{dX}{dx} = -\frac{X}{Q}\frac{dQ}{dx} + \frac{Q_S X_S}{Q} + \frac{Q_G X_G}{Q} + \frac{LA}{RQ} \qquad (3.14)$$

Since

$$\frac{dQ}{dx} = Q_S + Q_G$$

and

$$dx = \bar{V}\, d\tau$$

letting

$$Q = \bar{V}A$$

in a reach where

$\bar{V}$ = average reach velocity

then

$$\frac{dX}{d\tau} = \frac{-X(Q_S + Q_G)}{A} + \frac{Q_S X_S + Q_G X_G}{A} + \frac{L}{R}$$

or

$$\frac{dX}{d\tau} = \frac{Q_S(X_S - X) + Q_G(X_G - X)}{A} + \frac{L}{R} \qquad (3.15)$$

in which

τ = travel time (sec)

When Equation 3.15 is applied to a nonconservative constituent and to a reach with average cross-sectional area $\bar{A}$ and average hydraulic radius $\bar{R}$, it becomes:

$$\frac{dX}{d\tau} = \alpha + \frac{L}{\bar{R}} + \frac{Q_S(X_S - X) + Q_G(X_G - X)}{\bar{A}} \qquad (3.16)$$

in which

α = rate of loss or gain of the constituent due to biological reactions, physical removal, or phase transfers (mg/ℓ/sec)

For simplicity, the last two terms of Equation 3.16 can be expressed as:

$$S = \frac{L}{\bar{R}} + \frac{(S_S + S_G)}{\bar{A}} \qquad (3.17)$$

in which

$$S_S = \begin{cases} Q_S(X_S - X) & : \text{Flow into reach; } Q_S \text{ positive} \\ 0 & : \text{Flow out of reach; } Q_S \text{ negative} \end{cases}$$

$$S_G = \begin{cases} Q_G(X_G - X) & : \text{Flow into reach; } Q_G \text{ positive} \\ 0 & : \text{Flow out of reach; } Q_G \text{ negative} \end{cases}$$

so Equation 3.16 becomes:

$$\frac{dX}{d\tau} = \alpha + S \qquad (3.18)$$

Constituent equations

In theory, the solution technique used to determine the joint probability density function of state variables (to be described in a later section) is applicable for a system of n random differential equations. However, because of computer memory storage limitations, the technique is impractical for a system of greater than two equations. For this reason, PSSAM can simulate only two water quality constituents simultaneously. Although it has been noted in the literature [*EPA* 1973] that BOD-DO models have been overemphasized in the past, these constituents were chosen for this study because: 1) although overemphasized, the coupled BOD-DO systems are still important measures of water quality, and 2) data on the uncertainties associated with BOD and DO are more readily available than for any other constituents. The deterministic equations for BOD and DO are described below, and therein $\dot{X}_i$ is the derivative of the ith constituent with respect to the travel time τ.

BOD (Biochemical oxygen demand). The rate of change in BOD concentration is determined by the rates of first-order decay, first-order removal (settling, etc.), and mass input from diffuse sources and benthic leaching. In the nomenclature used below the first subscript indicates the constituent and the second designates the various types of model coefficients.

$$\dot{X}_1 = -\beta_{1,1}X_1 - \beta_{1,2}X_1 + S_1 \qquad (3.19)$$

in which

X_1 = concentration of BOD (mg/ℓ)

$\beta_{1,1}$ = first-order BOD decay rate (1/sec)

$\beta_{1,2}$ = first-order BOD removal rate (1/sec)

S_1 = net rate of mass input from lateral and benthic sources of BOD (mg/ℓ/sec)

DO (Dissolved oxygen). The rate of change in DO concentration is determined by the rates of reaeration across the surface, biochemical oxygen demand, photosynthetic production by algae, uptake by benthic deposits, and mass input from lateral inflow:

$$\dot{X}_2 = \beta_{2,1}(\beta_{2,2} - X_2) - \beta_{1,1}X_1 + \beta_{2,3} - \beta_{2,4}X_2/\bar{R} + S_2 \qquad (3.20)$$

in which

X_2 = concentration of DO (mg/ℓ)

$\beta_{2,1}$ = reaeration rate (1/sec)

$\beta_{2,2}$ = dissolved oxygen saturation at 20°C (mg/ℓ)

$\beta_{2,3}$ = net oxygen production by phytoplankton (mg/ℓ/sec)

$\beta_{2,4}$ = benthic uptake of oxygen ($g/m^2/sec/(mgO_2/ℓ)$)

S_2 = diffuse and benthic sources of DO (mg/ℓ/sec)

The reaeration coefficient ($\beta_{2,1}$) was calculated by

using the following equation [*Bishop and Grenney* 1977]:

$$\beta_{2,1} = 5.58\ \bar{V}^{0.607}/H^{1.689} \qquad (3.21)$$

in which

$\bar{V}$ = average velocity (m/sec)

H = depth (approximated by average hydraulic radius, $\bar{R}$) (m)

The dissolved oxygen saturation corrected for stream temperature and elevation was calculated using the following equation [*Bishop and Grenney* 1977]:

$$\beta_{2,2}(T_f,E) = \left[24.8 - 0.4259T_f + 0.003734T_f^2 - 0.00001328T_f^3\right]\left[\text{EXP}\left\{\frac{0.03419E}{288.0 - 0.006496E}\right\}\right] \qquad (3.22)$$

in which

T_f = stream temperature (°F)

E = elevation (m)

$\beta_{2,2}(T_f,E)$ = dissolved oxygen saturation at temperature T and elevation E (mg/ℓ)

Temperature correction

The BOD decay coefficient $\beta_{1,1}$ and the reaeration coefficient $\beta_{2,1}$ are temperature adjusted using the equation:

$$\beta_T = \beta_{20}\theta^{T-20} \qquad (3.23)$$

in which

β_T = coefficient at temperature T

β_{20} = coefficient at 20°C

T = stream temperature (°C)

θ = 1.047 for $\beta_{1,1}$, 1.0159 for $\beta_{2,1}$ [*Bishop and Grenney* 1977]

Matrix form of deterministic water quality equations

Substituting Equation 3.17 into Equations 3.19 and 3.20, and rearranging yields, respectively:

$$\dot{X}_1 = -(\beta_{1,1} + \beta_{1,2} + q)X_1 + (L_1/\bar{R} + q_S X_{S_1} + q_G X_{G_1}) \qquad (3.24)$$

$$\dot{X}_2 = -\beta_{1,1}X_1 - (\beta_{2,1} + \beta_{2,4}/\bar{R} + q)X_2 + (\beta_{2,1}\beta_{2,2} + \beta_{2,3} + L_2/\bar{R} + q_S X_{S_2} + q_G X_{S_2}) \qquad (3.25)$$

in which

$$q_S = Q_S/\bar{A} \qquad (3.26)$$

$$q_G = Q_G/\bar{A} \qquad (3.27)$$

$$q = q_S + q_G \qquad (3.28)$$

Rewriting Equations 3.24 and 3.25 in matrix form:

$$\begin{bmatrix}\dot{X}_1\\ \dot{X}_2\end{bmatrix} = \begin{bmatrix}-(\beta_{1,1} + \beta_{1,2} + q) & 0\\ -\beta_{1,1} & -(\beta_{2,1} + \beta_{2,4}/\bar{R} + q)\end{bmatrix}\begin{bmatrix}X_1\\ X_2\end{bmatrix} + \begin{bmatrix}L_1/\bar{R} + q_S X_{S_1} + q_G X_{G_1}\\ \beta_{2,1}\beta_{2,2} + \beta_{2,3} + L_2/\bar{R} + q_S X_{S_2} + q_G X_{G_2}\end{bmatrix} \qquad (3.29)$$

or

$$\dot{\underline{X}} = A\underline{X} + \underline{U} \qquad (3.30)$$

where A now represents a 2 × 2 matrix of constant coefficients and $\underline{U}$ is a vector of inputs to the system. In Equation 3.30, one has a system of deterministic differential equations describing the change in concentration of BOD and DO with travel time.

Random Water Quality Equations

The next step is to recast the deterministic equations as random differential equations by adding terms to account for the variability in the reaction rate coefficients and inputs.

Uncertainty in the coefficients

The manner in which the randomness in a coefficient is represented in the differential equations has a subtle yet important effect on the solution of the equation. Consider the following two cases:

$$\frac{dX(\tau)}{dt} = -CX(\tau), \quad C \sim N(K,1.0) \qquad (3.32)$$

$$\frac{dY(\tau)}{dt} = -(K+W(\tau))Y(t), \quad W(\tau) \sim N(0,1.0) \qquad (3.33)$$

C is a constant coefficient whose value is obtained from a normal distribution with mean K and variance 1.0. The value for C remains constant for each sample function. $W(\tau)$ is a zero mean Gaussian white noise process with a variance of 1.0. $W(\tau)$ changes with respect to travel time in each sample function. Some possible sample functions of Equations 3.32 and 3.33 are shown in Figures 3.3 and 3.4, respectively. The sample functions of Equation 3.32 are smooth curves while the sample functions of Equation 3.33 have a "noisy" path.

A possible physical interpretation of the differences between Equations 3.32 and 3.33 might proceed as follows. Each sample function of Equation 3.32 reflects the error in the estimation or determination of the coefficient. At the time of interest, the coefficient is assumed to have a constant but unknown value. For case 2 (Equation 3.33) the sample functions represent the effects of random fluctuations in the coefficients along the length of the stream. Thus case 2 appears to be closer to experience.

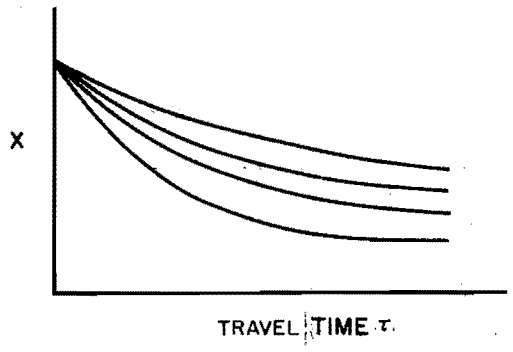


Figure 3.3. Sample functions of Equation 3.32.

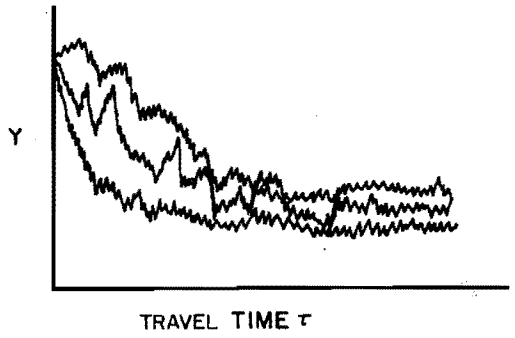


Figure 3.4. Sample functions of Equation 3.33.

In terms of the mathematical properties of the random coefficients, the two representations presented above are essentially two extremes of the spectrum. Case 1 (Equation 3.32) implies that the coefficients do not vary along the stream channel. Case 2 (Equation 3.33) corresponds to a coefficient that varies randomly about its mean as a function of travel time or distance along the channel. *Tsokos and Tsokos* [1976] state that the mean of the sample functions of Equation 3.32 is the deterministic solution. *Soong* [1971], however, shows that in general this is not true. The mean of the distribution of sample functions of Equation 3.33 is, however, the deterministic solution [*Soong* 1973]. Case 2 may be more appealing than Case 1 since one may intuitively expect the mean of a random process to be the deterministic solution. When input and initial condition randomness are also present, the second case of randomness in the coefficients may be more appealing than the first case since the resulting random differential equation is much easier to solve [*Soong* 1973]. Therefore, based on both mathematical and physical interpretations, the uncertainty in the water quality equation reaction rate coefficients ($\beta_{1,1}$, $\beta_{1,2}$, $\beta_{2,1}$, and $\beta_{2,4}$) was represented by a Gaussian white noise process having the form of Equation 3.33.

Uncertainty in the inputs

To account for natural random fluctuations and errors in measurement, the uncertainty in the inputs was represented by a Gaussian white noise process. The inputs which were considered to be random variables include the benthic leaching rates for BOD and DO (L_1 and L_2, respectively), the concentration of BOD and DO in the lateral surface and subsurface inflow (X_{S_1}, X_{S_2}, X_{G_1}, and X_{G_2}, respectively) and net oxygen production by phytoplankton ($\beta_{2,3}$).

Formulation of random water quality equations

Since the uncertainty in both the inputs and coefficients is represented by a Gaussian white noise process, Equation 3.30 can be transformed to a system of Ito differential equations. This is done by simply adding to Equation 3.30 a white noise term for each random input and coefficient. If WC denotes the noise process associated with the input or coefficient C, the system of Ito differential equations for BOD and DO can be written as follows:

$$\dot{\underline{X}} = A\underline{X} + \underline{U} + G\underline{W} \tag{3.34}$$

in which

$$G = \tag{3.35}$$

$$\begin{bmatrix} -X_1 & -X_1 & 0 & 0 & 1/\bar{R} & q_S & q_G & 0 & 0 & 0 & 0 \\ -X_1 & 0 & (-X_2 + \beta_{2,2}) & -X_2/\bar{R} & 0 & 0 & 0 & 1/\bar{R} & q_S & q_G & 1 \end{bmatrix}$$

$$\underline{W} = \begin{bmatrix} W\beta_{1,1} \\ W\beta_{1,2} \\ W\beta_{2,1} \\ W\beta_{2,4} \\ WL_1 \\ WX_{S_1} \\ WX_{G_1} \\ WL_2 \\ WX_{S_2} \\ WX_{G_2} \\ W\beta_{2,3} \end{bmatrix} \tag{3.36}$$

The vector $\underline{W}$ has the following properties:

$$E[\underline{W}(t)] = \underline{0} \tag{3.37}$$

$$E[\underline{W}(t)\underline{W}^t(s)] = \underline{Q}\delta(t-s) \tag{3.38}$$

where $\underline{Q}$ is the covariance parameter matrix and $\delta(t-s)$ is the Dirac delta function. If it can be assumed that the white noise processes are mutually independent, $\underline{Q}$ is a diagonal matrix with the diagonal terms, VC, equal to the variance parameter (variance per unit time) of the white noise process WC:

$$\text{diag}\,(\underline{Q}) = \tag{3.39}$$

$$(V\beta_{1,1}\ V\beta_{1,2}\ V\beta_{2,1}\ V\beta_{2,4}\ VL_1\ VX_{S_1}\ VX_{G_1}\ VL_2\ VX_{S_2}\ VX_{G_2}\ V\beta_{2,3})$$

While not absolutely necessary, the assumption that the white noise processes are mutually independent greatly simplifies the solution to Equation 3.34. If the noise processes being modeled are determined to be correlated, this assumption may be a major model limitation. The determination of two coefficients or inputs from the measurement of one variable is an example of a situation where correlated noise could occur. Further research is necessary to determine whether the independence assumption would introduce a significant error in the model estimates if the noise processes are not independent.

Several variables in Equation 3.30 are not considered to be random variables even though they may in fact be so. It was necessary to consider some variables as deterministic so that Equation 3.34 could be solved. If these variables had been considered to be random variables, multiplicative white noise terms would have occurred in Equation 3.34, but a technique for solving Ito differential equations with multiplicative white noise terms has not yet been developed. The deterministic variables are the streamflow (Q), the lateral surface and subsurface inflows (Q_S and Q_G) and the dissolved oxygen saturation concentration ($\beta_{2,2}$). The choice of the flow variables as the deterministic variables was based on a convenient separation of the flow and water quality variables and coefficients (except $\beta_{2,2}$) into deterministic and random variables, respectively. Thus the joint pdf of BOD and DO is conditioned on the flows which are assumed known without error. Either $\beta_{2,1}$ or $\beta_{2,2}$ could be treated as a random variable since they appear in multiplicative form in Equation 3.25. However, evidence in the literature points to $\beta_{2,1}$, the reaeration rate, having greater variability about its mean than $\beta_{2,2}$, the DO saturation concentration, and on this basis $\beta_{2,2}$ was treated as a deterministic variable. Further work should be directed to examining the optimal combination of deterministic and random variables which maximizes the amount of the prediction uncertainty which is represented under the constraint of not being able to treat random variables in multiplicative terms.

Another limitation of treating the randomness in the inputs and coefficients of the water quality equations as white noise processes is that only time independent randomness can be considered. This eliminates the consideration of the dynamic fluctuations in point load flow and quality (*i.e.*, wastewater treatment plants) and the diurnal cycle of many aquatic processes (for example oxygen production by phytoplankton). However, this limitation is consistent with the steady-state assumption that is made for the deterministic portion of the model.

Fokker-Plank equation

$\underline{X}$, the solution to an Ito differential equation, is a Markov process [*Soong* 1973]. Therefore $f_{\underline{X}}(\underline{X},\tau)$, the joint probability density function (pdf) of $\underline{X}$, can be found using the Fokker-Plank Equation (also known as the Forward Kolmogorov Diffusion Equation) [*Soong* 1973], below:

$$\frac{\partial f_{\underline{X}}(\underline{X},\tau)}{\partial \tau} = -\sum_{j=1}^{2} \frac{\partial}{\partial X_j}\left[(A_j\underline{X} + U_j)f\right] + \tfrac{1}{2}\sum_{j=1}^{2}\sum_{i=1}^{2} \frac{\partial^2}{\partial X_i X_j}\left[(G\underline{W}G^t)_{ij} f\right] \tag{3.40}$$

in which A_j is the jth row of matrix A, U_j is the jth entry of the vector $\underline{U}$, $(G\underline{W}G^t)_{ij}$ is the ijth entry of the matrix $(G\underline{W}G^t)$, X_j is the jth entry of the vector $\underline{X}$ and $f_{\underline{X}}(\underline{X},\tau)$ is abbreviated to f for compactness of the notation. In order to completely specify the problem it is assumed that the initial probability density function, $f_{\underline{X}}(\underline{X}_0,\tau_0)$ is known and that the boundary condition for Equation 3.40 is $f_{\underline{X}}(\pm\infty,\tau_0) = 0$ for all τ. By specifying $f_{\underline{X}}(\underline{X}_0,\tau_0)$ at headwaters and point loads, the joint pdf of BOD and DO can be determined at any location in the stream using Equation 3.40.

PDF of Headwater and Point Loads

The concentrations of BOD and DO at the headwater and in the point loads were assumed to have a bivariate normal distribution. However, with minor program modifications, any bivariate distribution could be considered.

Determination of PDF Downstream of Point Load

The joint pdf of BOD and DO immediately downstream of a point load was determined by convoluting the upstream river and point load probability density functions. Assuming complete and instantaneous mixing of the river and point load flows, the random variables X_1 and X_2, the concentrations of BOD and DO, respectively, immediately downstream of the point load can be defined as follows:

$$X_1 = (Q_u X_{1_u} + Q_\ell X_{1_\ell})/(Q_u + Q_\ell) \tag{3.41}$$

$$X_2 = (Q_u X_{2_u} + Q_\ell X_{2_\ell})/(Q_u + Q_\ell) \tag{3.42}$$

in which

X_{1_u} = concentration of BOD immediately upstream of point load (mg/ℓ)

X_{2_u} = concentration of DO immediately upstream of point load (mg/ℓ)

X_{1_ℓ} = concentration of BOD in point load (mg/ℓ)

X_{2_ℓ} = concentration of DO in point load (mg/ℓ)

Q_u = flow immediately downstream of point load (m^3/sec)

Q_ℓ = flow of point load (m^3/sec)

If we let

$$\alpha = Q_u/(Q_u + Q_\ell) \tag{3.43}$$

$$\gamma = Q_\ell/(Q_u + Q_\ell) \tag{3.44}$$

then

$$X_1 = \alpha X_{1_u} + \gamma X_{1_\ell} \tag{3.45}$$

$$X_2 = \alpha X_{2_u} + \gamma X_{2_\ell} \tag{3.46}$$

By the method of derived distributions it is shown in the Appendix that the joint pdf of BOD and DO downstream of a point load is given by:

$$f_{X_1X_2}(x_1x_2) = \frac{1}{\alpha^2}\int_{X_{1_\ell}}\int_{X_{2_\ell}} f_{X_{1_u}X_{2_u}}\left(\frac{x_1-\gamma x_{1_\ell}}{\alpha}\ \frac{x_2-\gamma x_{2_\ell}}{\alpha}\right) f_{X_{1_\ell}X_{2_\ell}}(x_{1_\ell}x_{2_\ell})\,dX_{1_\ell}dX_{2_\ell} \tag{3.47}$$

Moment Equations

Two important characteristics of a bivariate probability distribution are its mean vector and covariance matrix. Although they could be determined by numerical integration of the pdf, it would be computationally more efficient to derive a set of moment equations from which the mean vector and covariance matrix could be calculated. *Soong* [1973] showed that it is possible to derive a set of differential equations which satisfy the moments of the solution process of Equation 3.34. These moment equations are of the form:

$$\frac{d}{d\tau}\,E\,[h(\underline{X},\tau)] = \sum_{j=1}^{2} E[(A_j\underline{X} + U_j)(\partial h/\partial X_j)] + \tfrac{1}{2}\sum_{j=1}^{2}\sum_{i=1}^{2} E[(G\underline{Q}G^t)_{ij}\partial^2 h/\partial X_i\partial X_j] + E[\partial h/\partial\tau] \tag{3.48}$$

where $h(\underline{X},\tau)$ is an arbitrary function of $\underline{X}$ and τ. The first moment equation can be derived by letting $h(\underline{X},\tau) = E(\underline{X})$. The first and second moment equations for $\underline{X}$ are given in Table 3.1. Note that the derivatives are with respect to the travel time τ and that a_{ij} is the ijth entry of matrix A and U_i is the ith entry in vector $\underline{U}$. Equations for the entries of the covariance matrix (Γ) of $\underline{X}$, derived from the equations in Table 3.1 are as follows:

$$\dot{\Gamma}_{11} = 2a_{11}\Gamma_{11} + (V\beta_{1,1} + V\beta_{1,2})[\Gamma_{11} + E^2(X_1)] + VL_1/\bar{R}^2 + q_S^2VX_{S_1} + q_G^2VX_{G_1} \tag{3.49}$$

$$\dot{\Gamma}_{12} = \dot{\Gamma}_{21} = a_{21}\Gamma_{11} + (a_{11} + a_{22})\Gamma_{12} + V\beta_{1,1}[\Gamma_{11} + E^2(X_1)] \tag{3.50}$$

$$\dot{\Gamma}_{22} = 2a_{21}\Gamma_{12} + 2a_{22}\Gamma_{22} + V\beta_{1,1}[\Gamma_{11} + E^2(X_1)] + 2(V\beta_{2,1} + V\beta_{2,4}/\bar{R}^2)[\Gamma_{22} + E^2(X_2)] - 2E(X_2)\beta_{2,2}V\beta_{2,1} + \beta_{2,2}^2V\beta_{2,1} + V\beta_{2,3} + VL_2/\bar{R}^2 + q_S^2VX_{S_2} + q_G^2VX_{G_2} \tag{3.51}$$

The first moment equations in Table 3.1 and Equations 3.49 through 3.51 were used in the model PSSAM to calculate the mean and variance of BOD [$E(X_1)$ and Γ_{11}, respectively], the mean and variance of DO [$E(X_2)$ and Γ_{22}, respectively], and the covariance of BOD and DO (Γ_{12}).

The moment equations shown in Table 3.1 are of the form:

$$\dot{\underline{M}} = \phi\underline{M} + \underline{L} \tag{3.52}$$

If there are no repeated roots, every solution $M(t)$ of the homogeneous part of Equation 3.52 is of the form:

$$\underline{M}(t) = \sum_{i=1}^{5} (c_i e^{\lambda_i t}\underline{V}_i) \tag{3.53}$$

where c_i is a constant and $\underline{V}_i$ is an eigenvector of ϕ with eigenvalue λ_i. Note that the eigenvalues of ϕ are the diagonal entries since ϕ is triangular. It is often desirable for the mean vector and covariance matrix to be asymptotically stable (approach some equilibrium value as τ approaches infinity). Since a_{11} and a_{22} are always negative, the mean vector will always be asymptotically stable. It can be shown from Equation 3.53 that a necessary and sufficient condition for the asymptotic stability of the second moments of $\underline{X}$ is that all the eigenvalues of ϕ be negative. Since a_{11} and a_{22} are negative, this condition implies that the following inequalities are satisfied:

$$V\beta_{1,1} + V\beta_{1,2} < 2(\beta_{1,1} + \beta_{1,2} + q) \tag{3.54}$$

$$V\beta_{2,1} + V\beta_{2,4}/\bar{R}^2 < 2(\beta_{2,1} + \beta_{2,4}/\bar{R} + q) \tag{3.55}$$

It is convenient to assume that VC, the standard deviation parameter of the noise associated with input or coefficient C is equal to some fraction $0 \le K_C \le 1$ of C

$$VC = K_C C \tag{3.56}$$

If the coefficients $\beta_{1,1}$, $\beta_{1,2}$, $\beta_{2,1}$, and $\beta_{2,4}/\bar{R}$ all have numerical values less than 1.0, Equations 3.54 and 3.55 will be satisfied for any K_C. If any one of the four coefficients has a numerical value greater than 1.0, Equations 3.54 and 3.55 provide a means of calculating an upper bound on K_C for which the covariance matrix will remain asymptotically stable.

Table 3.1. First and second moment equations for BOD and DO.

$$\begin{bmatrix} \dot{E}(X_1) \\ \dot{E}(X_2) \\ \dot{E}(X_1^2) \\ \dot{E}(X_1X_2) \\ \dot{E}(X_2^2) \end{bmatrix} = \begin{bmatrix} a_{11} & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & 0 & 0 & 0 \\ 2U_1 & 0 & 2a_{11} + z_1 & 0 & 0 \\ U_2 & U_1 & a_{21} + V\beta_{1,1} & a_{11} + a_{22} & 0 \\ 0 & 2(U_2 - z_2) & V\beta_{1,1} & 2a_{21} & 2a_{22} + z_3 \end{bmatrix} \begin{bmatrix} E(X_1) \\ E(X_2) \\ E(X_1^2) \\ E(X_1X_2) \\ E(X_2^2) \end{bmatrix} + \begin{bmatrix} U_1 \\ U_2 \\ I_3 \\ 0 \\ I_5 \end{bmatrix}$$

where

$$z_1 = V\beta_{1,1} + V\beta_{1,2}$$

$$z_2 = \beta_{2,2}\, V\beta_{2,1}$$

$$z_3 = V\beta_{2,1} + V\beta_{2,4}/\bar{R}^2$$

$$I_3 = VL_1/\bar{R}^2 + q_S^2 VX_{S_1} + q_G^2 VX_{G_1}$$

$$I_5 = \beta_{2,2}^2 V\beta_{2,1} + VL_2/\bar{R}^2 + q_S^2 VX_{S_2} + q_G^2 VX_{G_2} + V\beta_{2,3}$$

Numerical Solution Techniques

Determining the joint probability density function of BOD and DO requires finding a solution to the Fokker-Plank Equation (Equation 3.40). Unfortunately, except for when there is no coefficient noise, a closed form solution to Equation 3.40 has not been found. It is possible, however, to solve Equation 3.40 numerically.

Equation 3.40 can be classified as a mixed second-order parabolic partial differential equation in the variables τ (travel time), X_1 (BOD), and X_2 (DO). One of the best techniques for numerically solving parabolic partial differential equations with two space variables is the alternating-direction implicit (ADI) finite difference method first proposed by *Peaceman and Rachford* [1955]. The ADI method is unconditionally stable for any step size $\Delta\tau$ and is computationally efficient, but is not applicable to equations with mixed partial derivative terms. Therefore, to use the ADI method, the mixed partial derivative term in Equation 3.40 was eliminated using a technique described below.

If Z_Y denotes the partial derivative of Z with respect to Y and g_i and h_{ij} are defined as follows:

$$g_i = A_i \underline{X} + U_i \tag{3.57}$$

$$h_{ij} = [(G\underline{Q}G^t)_{ij}]/2 \tag{3.58}$$

then Equation 3.40 can be rewritten as:

$$f_\tau = Bf_{X_1^2} + 2Cf_{X_1X_2} + Df_{X_2^2} + Ef_{X_1} + Ff_{X_2} + Hf \tag{3.59}$$

in which

$$B = h_{11}$$

$$C = h_{12}$$

$$D = h_{22}$$

$$E = 2h_{11_{X_1}} - g_1$$

$$F = 2h_{12_{X_1}} + 2h_{22_{X_2}} - g_2$$

$$H = h_{11_{X_1^2}} + h_{22_{X_2^2}} - g_{1_{X_1}} - g_{2_{X_2}}$$

Consider a second-order linear partial differential operator $L(f)$ defined as follows:

$$L(f) \equiv Bf_{X_1^2} + 2Cf_{X_1X_2} + Df_{X_2^2} + Ef_{X_1} + Ff_{X_2} + Hf \tag{3.60}$$

If two new coordinates, P and S are given as functions of X_1 and X_2, then by using the chain rule of differentiation, it can be shown that in the new coordinate system:

$$\begin{aligned} L(f) \equiv\ & [B(P_{X_1})^2 + 2CP_{X_1}P_{X_2} + D(P_{X_2})^2]f_{P^2} \\ & + 2[BP_{X_1}S_{X_1} + CP_{X_1}S_{X_2} + CP_{X_2}S_{X_1} + DP_{X_2}S_{X_2}]f_{PS} \\ & + [B(S_{X_1})^2 + 2CS_{X_1}S_{X_2} + D(S_{X_2})^2]f_{S^2} \\ & + [L(P) - HP]f_P + [L(S) - HS]f_S + Hf \end{aligned} \tag{3.61}$$

The mixed partial derivative term in Equation 3.59 can be eliminated by choosing P and S so that the following differential equation is satisfied:

$$BP_{X_1}S_{X_1} + CP_{X_1}S_{X_2} + CP_{X_2}S_{X_1} + DP_{X_2}S_{X_2} = 0 \tag{3.62}$$

One choice for P and S that satisfies Equation 3.62 is:

$$P = X_1 \tag{3.63}$$

$$S = X_2 - \frac{V\beta_{1,1}}{V\beta_{1,1} + V\beta_{1,2}} \left[X_1 - (Z) \arctan\left(\frac{X_1}{Z}\right) \right] \quad (3.64)$$

in which

$$Z = \left[\frac{\frac{VL_1}{\bar{R}^2} + q_S^2 V X_{S_1} + q_G^2 V X_{G_1}}{V\beta_{1,1} + V\beta_{1,2}} \right]^{1/2} \quad (3.65)$$

Combining Equations 3.59, 3.61, 3.63, and 3.64 yields:

$$f_\tau = Bf_{P^2} + If_{S^2} + Ef_P + Jf_S + Hf \quad (3.66)$$

in which

$$I = D - C^2/B \quad (3.67)$$

$$J = (X_1/B)[C(V\beta_{1,1} + V\beta_{1,2}) - BV\beta_{1,1}] - EC/B + F \quad (3.68)$$

Equation 3.66 is solved by the ADI finite difference method in PSSAM. The joint pdf of BOD and DO (X_1 and X_2) is determined when necessary (*i.e.*, for printed output) by 10th-order Newton's divided-difference polynomial interpolation of f as a function of P and S using the transformation coordinate equations (Equations 3.63 and 3.64).

The differential equations for the mean vector and covariance matrix of $\underline{X}$ (the first two equations in Table 3.1 and Equations 3.49 through 3.51) were solved using a fourth-order Runge-Kutta algorithm. Equation 3.47, used to determine the joint pdf of BOD and DO immediately downstream of a point load, was solved using a 15 point Gauss-Legendre quadrature algorithm. The Newton's divided-difference interpolation algorithm, the Runge-Kutta algorithm, and the Gauss-Legendre algorithm were used because they are recognized to be computationally efficient and accurate.

Summary of Model Limitations

The probabilistic river water quality model developed herein has several limitations which were discussed as they came up in the above model formulation and are summarized below. Limitations resulting from treating the randomness in the inputs and coefficients of the water quality equations as white noise processes are as follows:

1. Only time independent randomness can be considered.
2. The white noise processes for inputs and coefficients are assumed to be independent.
3. Only linear white noise processes can be considered.

Model limitations resulting from simplifying assumptions and computer storage limitations are as follows:

1. Longitudinal dispersion in the river is assumed negligible.
2. Steady streamflow is assumed.
3. Mass transport is assumed to be one-dimensional.
4. All physiochemical characteristics of the river are assumed to be time invariate.
5. Mixing of a point load flow with the river is instantaneous and complete.
6. Only two state variables can be modeled. Changing the two state variables from BOD and DO would require extensive reprogramming.
7. Flows are treated as deterministic variables.
8. DO saturation, $\beta_{2,2}$, is treated as a deterministic variable which depends on only stream temperature and elevation according to Equation 3.22.
9. Equations used in the basic model are assumed to be correct and to completely describe the represented process.

CHAPTER IV

APPLICATIONS OF PROBABILISTIC RIVER WATER QUALITY MODEL

The probabilistic river water quality model PSSAM consisting of a programmed solution to Equation 3.66 was applied to a sensitivity problem and to a hypothetical river system. These two applications will be discussed in detail in sections to follow. In both applications, the headwater initial condition and point load effluent were assumed to be described by a bivariate normal distribution. A normal initial condition was used to be consistent with all the existing probabilistic water quality models reported in Chapter II. In the final section of this chapter the computational requirements of the model PSSAM will be summarized.

Sensitivity Problem

In order to gain familiarity with PSSAM, a sensitivity study was performed. The sensitivity of the model's predictions to changes in the input and coefficient noise variance parameter was investigated.

Problem description

A diagram of the section of river used in the sensitivity problem is given in Figure 4.1. It consists of a headwater and one reach with three check points. The data in Tables 4.1 through 4.3 provide the necessary input data used to study sensitivity. A summary of the river layout and hydraulics and a description of the five points at which the joint probability density function for BOD and DO is determined is given in Table 4.1. The mean vector and covariance matrix of the headwater quality are as follows:

$$\underline{X} = \begin{bmatrix} 15.0 \\ 5.0 \end{bmatrix}$$

$$\Gamma = \begin{bmatrix} 3.0 & 1.0 \\ 1.0 & 1.0 \end{bmatrix}$$

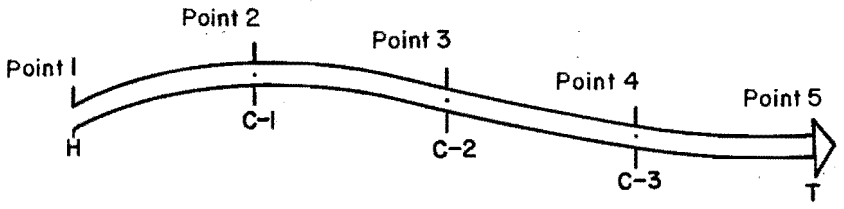


Figure 4.1. River layout for sensitivity problem.

Table 4.1. River system layout and hydraulics for sensitivity problem.

Point Number	Description	Location (km)	Input Flow (m^3/sec)	Lateral Inflow for Reach: Surface (m^3/sec/km)	Lateral Inflow for Reach: Ground (m^3/sec/km)	River Flow (m^3/sec)	Ave. Reach Vel. (m/sec)	H. Rad. (m)
1	Head of Reach	20.	5.0	0.02	0.02	5.0	0.25	3.39
2	Check Point 1	15.				5.2		
3	Check Point 2	10.				5.4		
4	Check Point 3	5.				5.6		
5	Termination	0				5.8		

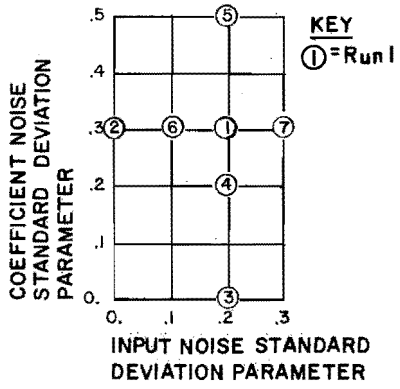
Table 4.2. Inputs, water temperature and water quality coefficients for sensitivity problem.

Constituent	Coefficient Symbol	Coefficient Units	Description	Coefficient Value
BOD	$\beta_{1,1}$	1/day	First-order decay rate	0.25[1]
	$\beta_{1,2}$	1/day	First-order removal rate	0.0
	L_1	g/m²/day	Leach rate	1.0
	X_{S_1}	mg/ℓ	Lateral surface inflow	10.0
	X_{G_1}	mg/ℓ	Lateral subsurface inflow	5.0
DO	$\beta_{2,1}$	1/day	Reaeration rate	0.65[1]
	$\beta_{2,2}$	km	Elevation	1.0
	$\beta_{2,3}$	mg/ℓ/day	Net oxygen production by phytoplankton	1.0
	$\beta_{2,4}$	$(g/m^2/day)/(mgO_2/\ell)$	Benthic uptake of oxygen	0.20
	L_2	g/m²/day	Leach rate	0.0
	X_{S_2}	mg/ℓ	Lateral surface inflow	3.0
	X_{G_2}	mg/ℓ	Lateral subsurface inflow	0.0
Temperature	T	°C	Water temperature	16.0

[1] Coefficient value is corrected to 20°C.

Table 4.3. Standard deviation parameters (K_c) for input and coefficient noise.

Run	Input Noise Standard Deviation Parameter (Fraction of Input)	Coefficient Noise Standard Deviation Parameter (Fraction of Coefficient)
1	0.2	0.4
2	0.0	0.4
3	0.2	0.0
4	0.2	0.3
5	0.2	0.5
6	0.1	0.4
7	0.3	0.4



where the units for $\underline{X}$ are mg/ℓ and the units for Γ are (mg/ℓ) . The value of the covariance between BOD and DO is consistent with the correlation between those variables recorded in the literature. The water quality equation coefficients and inputs are given in Table 4.2.

To assure that the sensitivity analysis was based on a reasonable representation of a river reach, many of the coefficients and input values used were taken from those reported by *Finney et al.* [1977] for portions of the Jordan River in Utah. The input and coefficient noise standard deviation parameters were assumed to be fractions of the respective input or coefficient values. In each of seven simulation runs, the fraction was varied. The standard deviation parameter of the water quality equation coefficient noise was varied between zero and 50 percent of the coefficient. This range seemed reasonable since *Kothandaraman and Ewing* [1969] found that the BOD first-order decay rate in the Ohio River was a normally distributed random variable with the standard deviation being 40 percent of the mean. The standard deviation parameter for the input noise was varied between zero and 30 percent of the input. This range was set arbitrarily because no values have been reported in the literature. The standard deviation parameter fractions for the input and coefficient noise used in each sensitivity run are summarized in Table 4.3. The same fraction was used for all inputs and all coefficients in each sensitivity run.

Results for sensitivity study

The sensitivity of the model predictions to input and coefficient noise was most apparent in sensitivity runs 1 through 3 so the discussion of the results will be confined to these runs. The joint pdf of BOD and DO at point 5 for run 1 is shown in Figure 4.2. Although it is of little quantitative use, it does help visualize the joint pdf. It can also be used to evaluate the stability of the numerical solution technique. A jagged surface could indicate numerical instability of the solution technique.

Figures 4.3 through 4.8 show the marginal pdf for BOD and DO at points 1 through 5 for each of the three runs. Examination of Figures 4.3 through 4.6 shows that the model response for runs 1 and 2 is nearly identical. This observation is substantiated by Figures 4.9 and 4.10 which show that the variance of BOD and DO for runs 1 and 2 is indistinguishable at all points. This would suggest that with the assumptions used in developing the model the coefficient noise contributes significantly more to the variance of the model predictions than does the input noise. Whether this would hold true for the broad range of coefficients and inputs found in river systems needs to be investigated. If this conclusion is found to be true in most river systems, then research efforts to quantify the standard deviation parameters of water quality equation coefficients should be intensified. It should be noted that this conclusion would not necessarily be expected to be true under unsteady conditions.

The pdf of BOD and DO in Figures 4.3 through 4.8 appears to be symmetric, suggesting that these variables could be approximated by a normal distribution. For example, the marginal cumulative distribution function (cdf) for BOD and DO at point 5 for run 2 is compared to those of normal distributions with the same means and variances in Figures 4.11 and 4.12. The probability of the

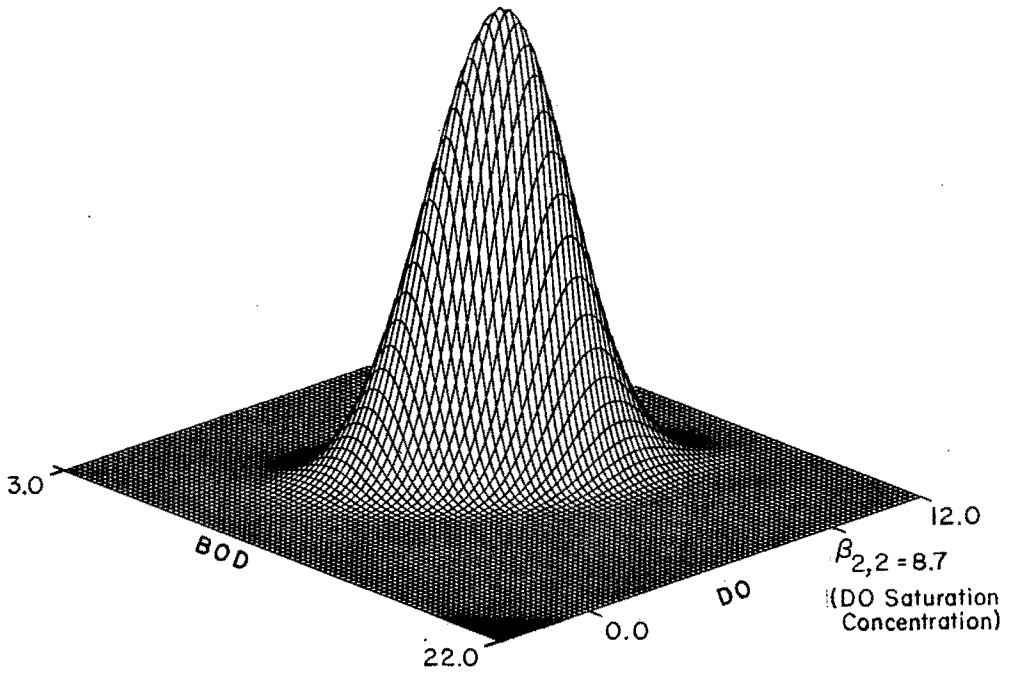


Figure 4.2. Joint pdf of BOD and DO at point 5 for run 1.

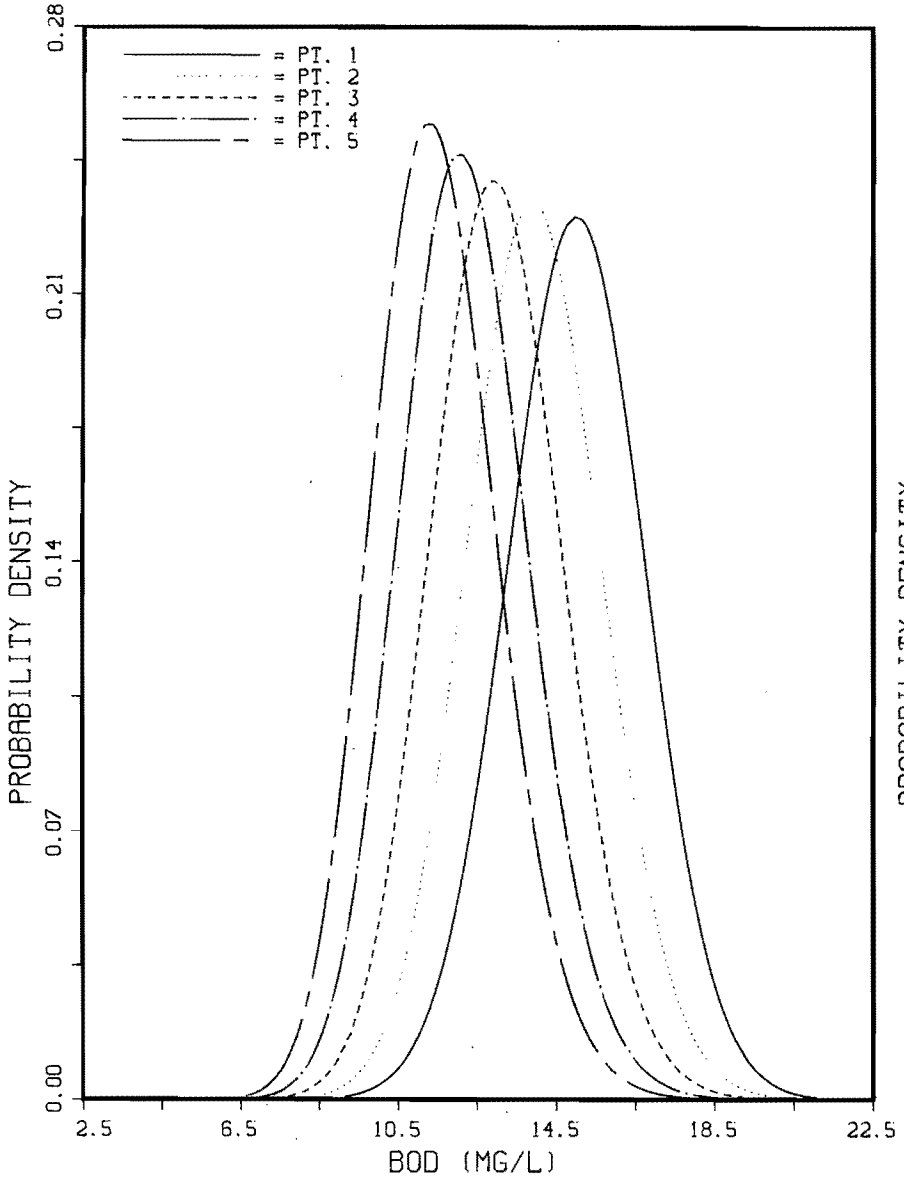


Figure 4.3. Marginal pdf of BOD at points 1 through 5 for run 1.

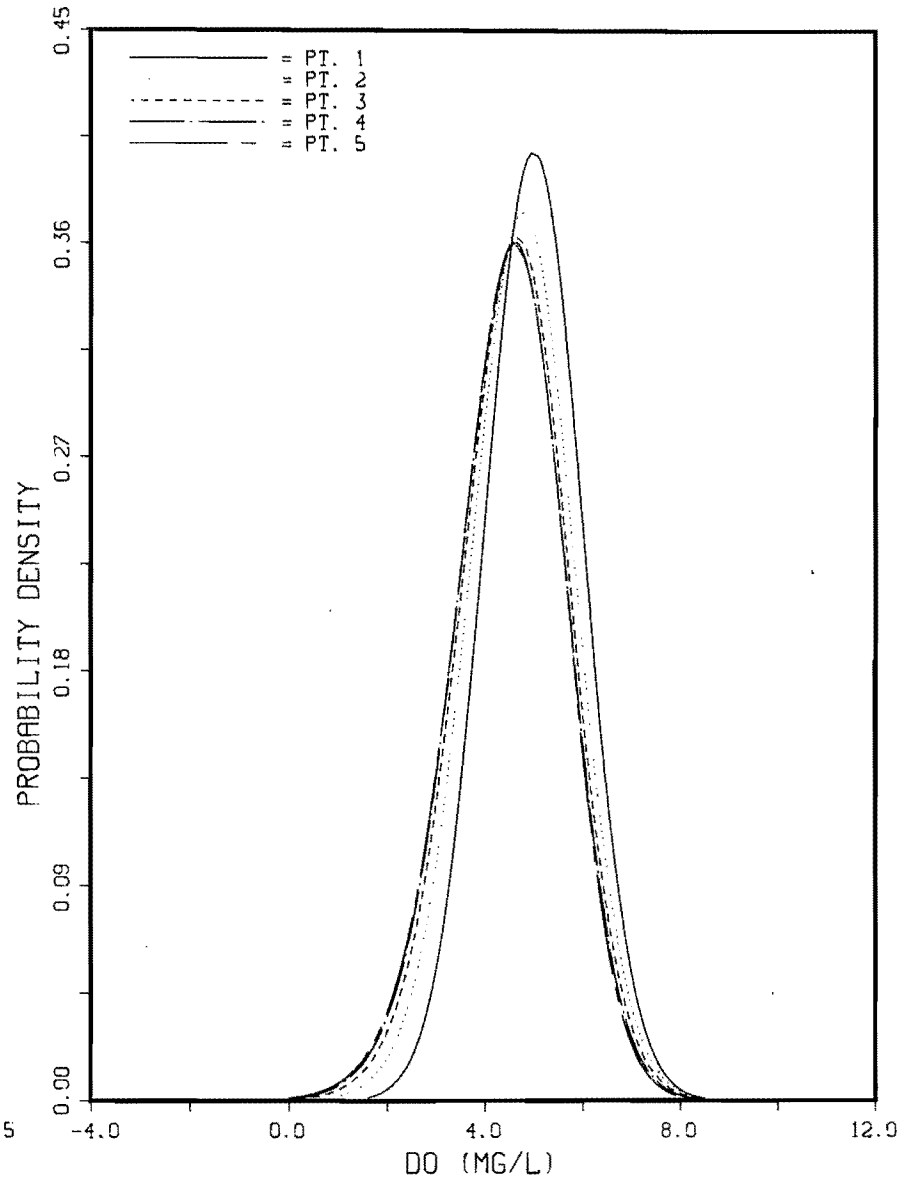


Figure 4.4. Marginal pdf of DO at points 1 through 5 for run 1.

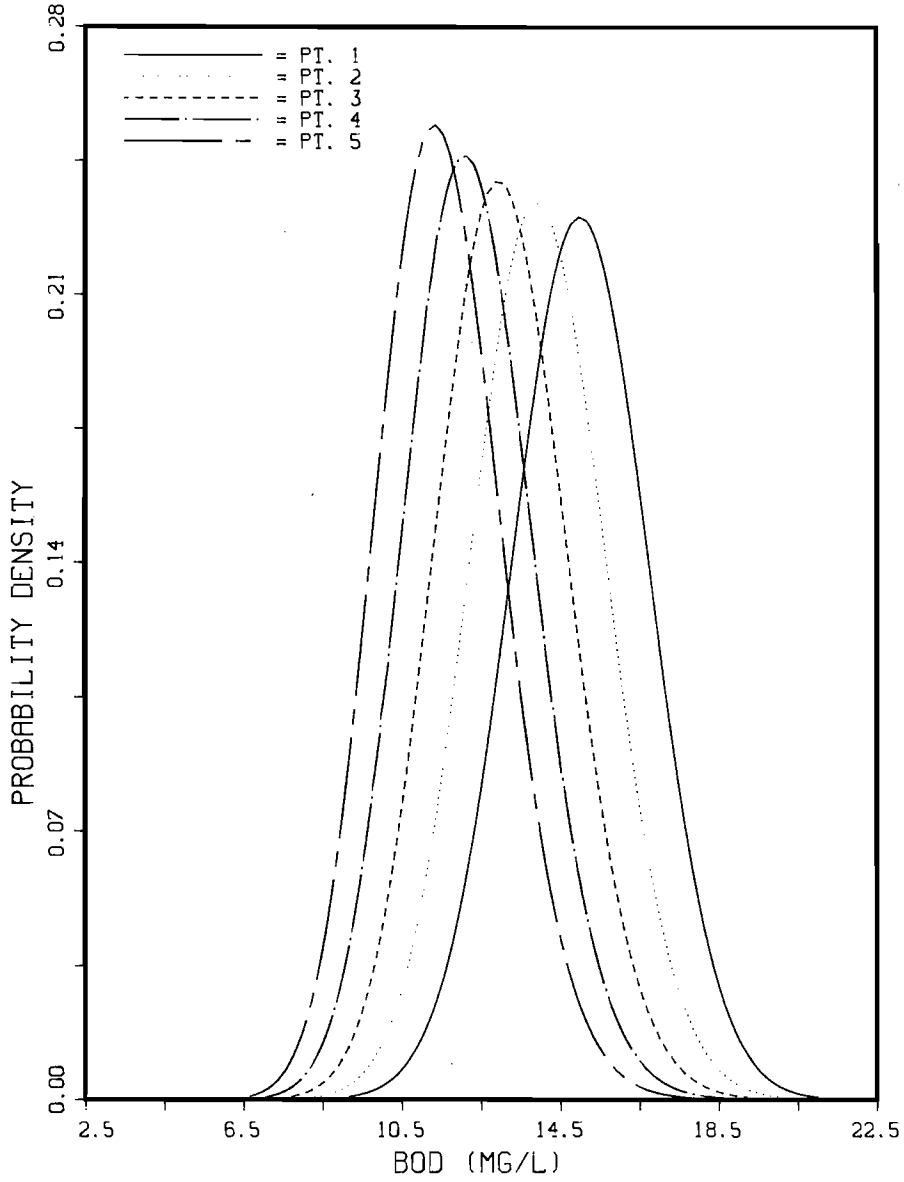


Figure 4.5. Marginal pdf of BOD at points 1 through 5 for run 2.

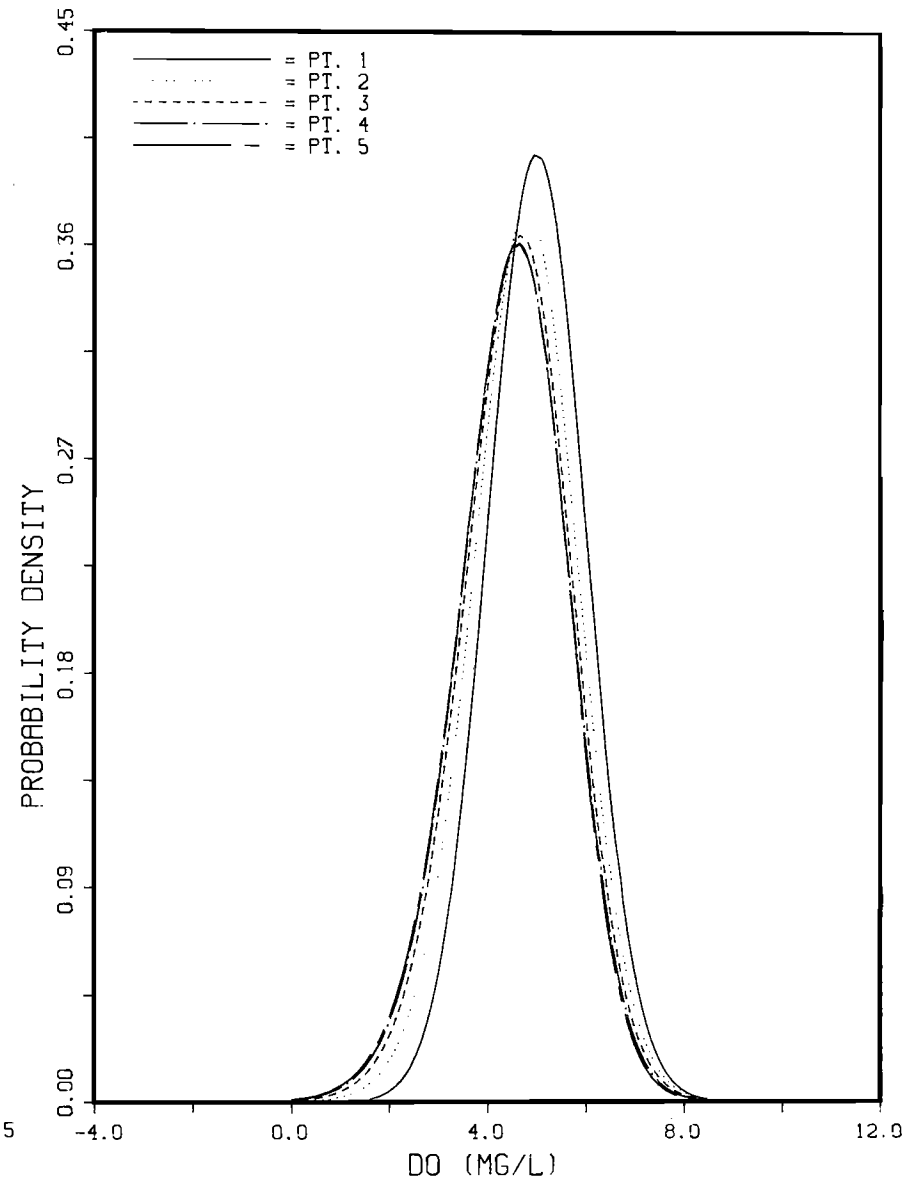


Figure 4.6. Marginal pdf of DO at points 1 through 5 for run 2.

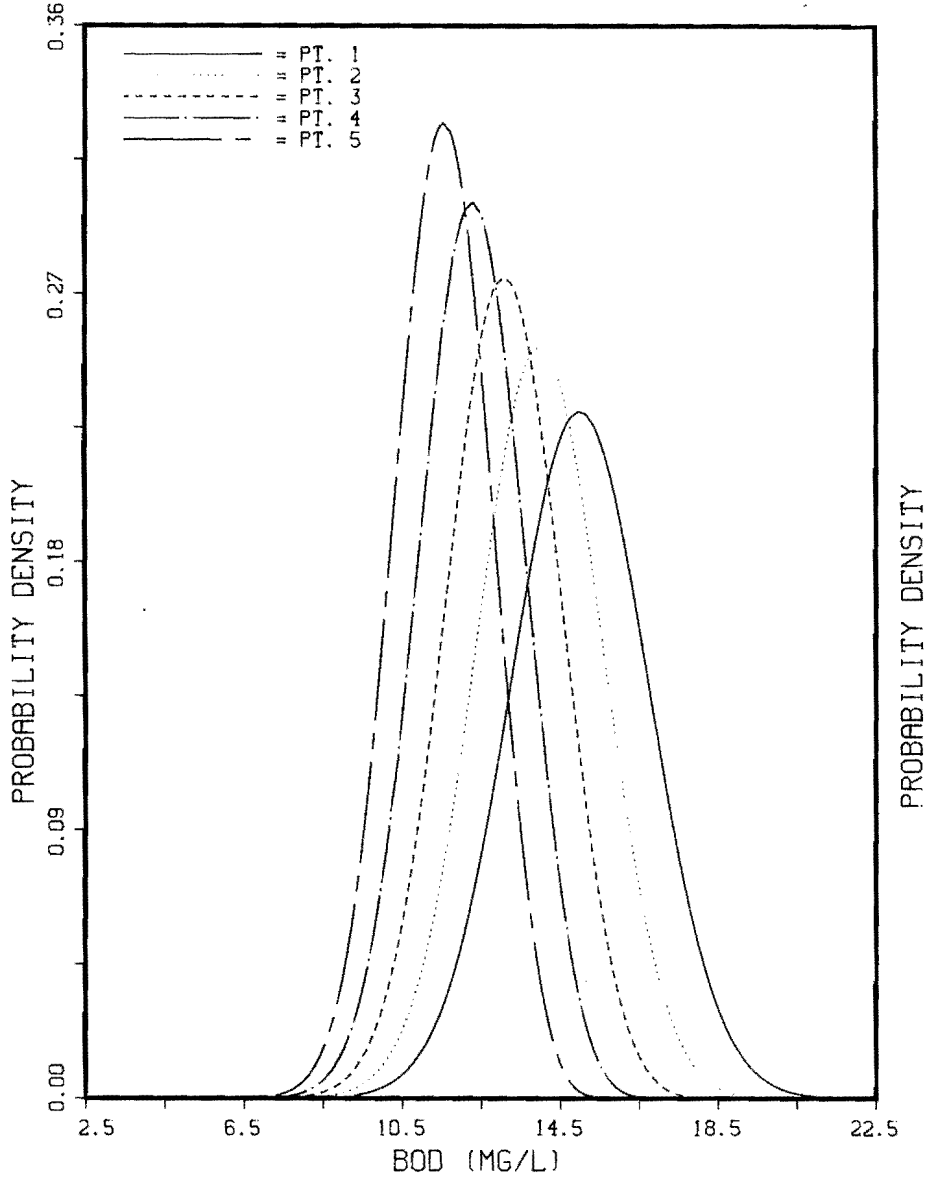


Figure 4.7. Marginal pdf of BOD at points 1 through 5 for run 3.

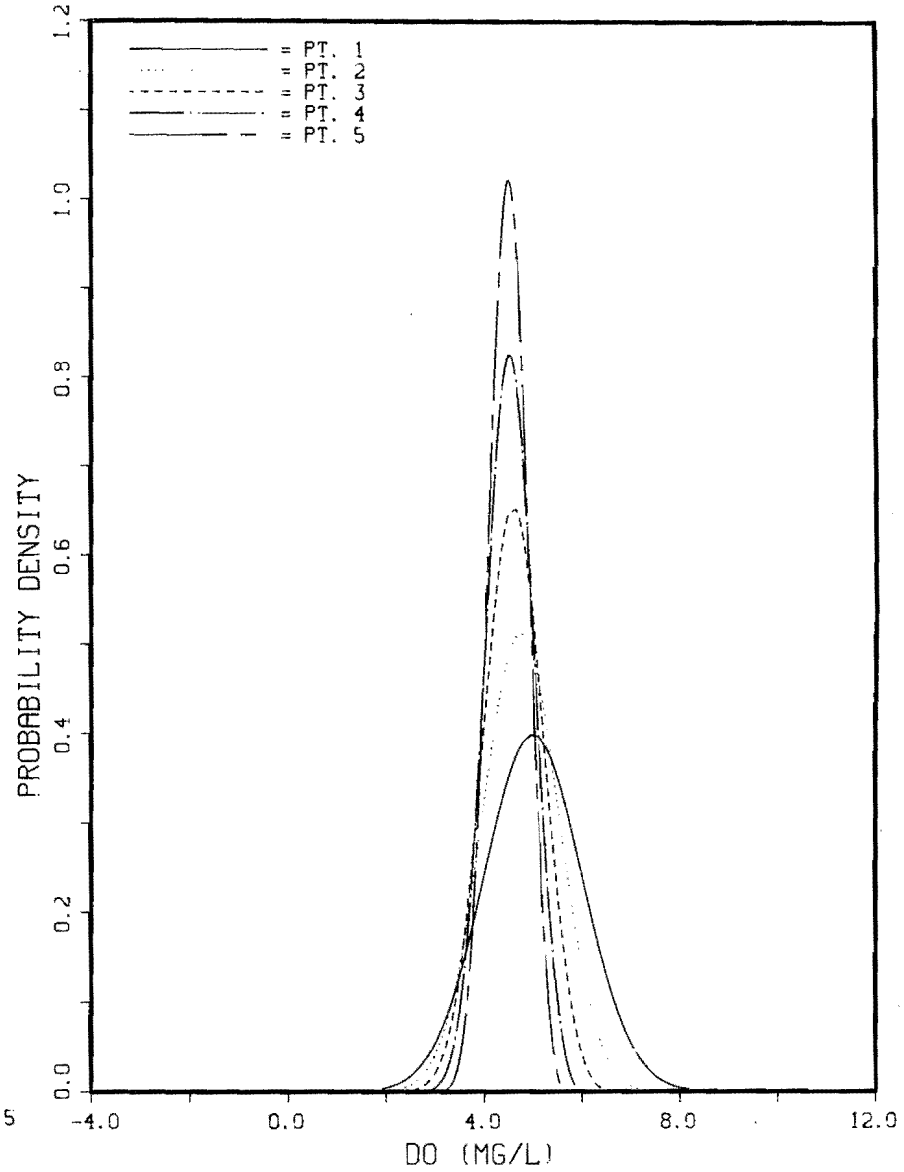


Figure 4.8. Marginal pdf of DO at points 1 through 5 for run 3.

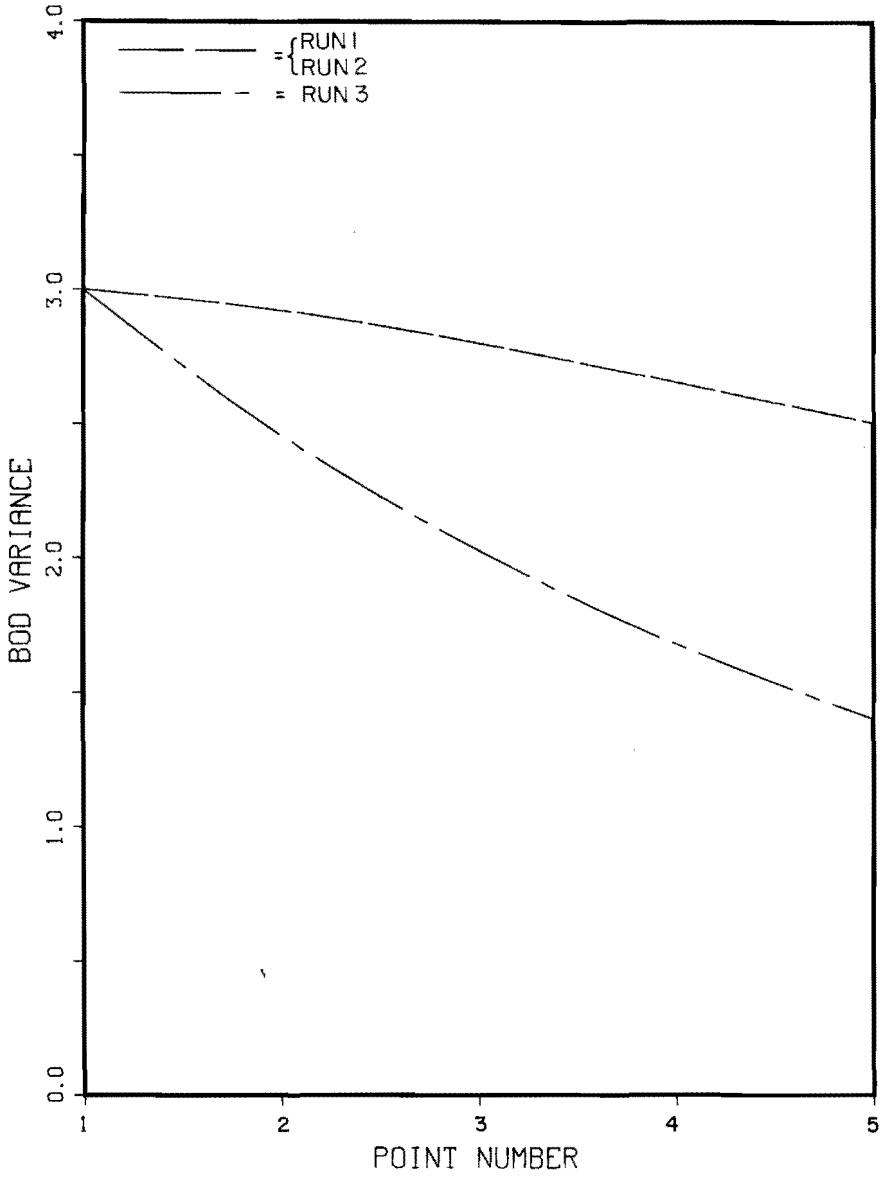


Figure 4.9. Variance of BOD at points 1 through 5 for runs 1 through 3.

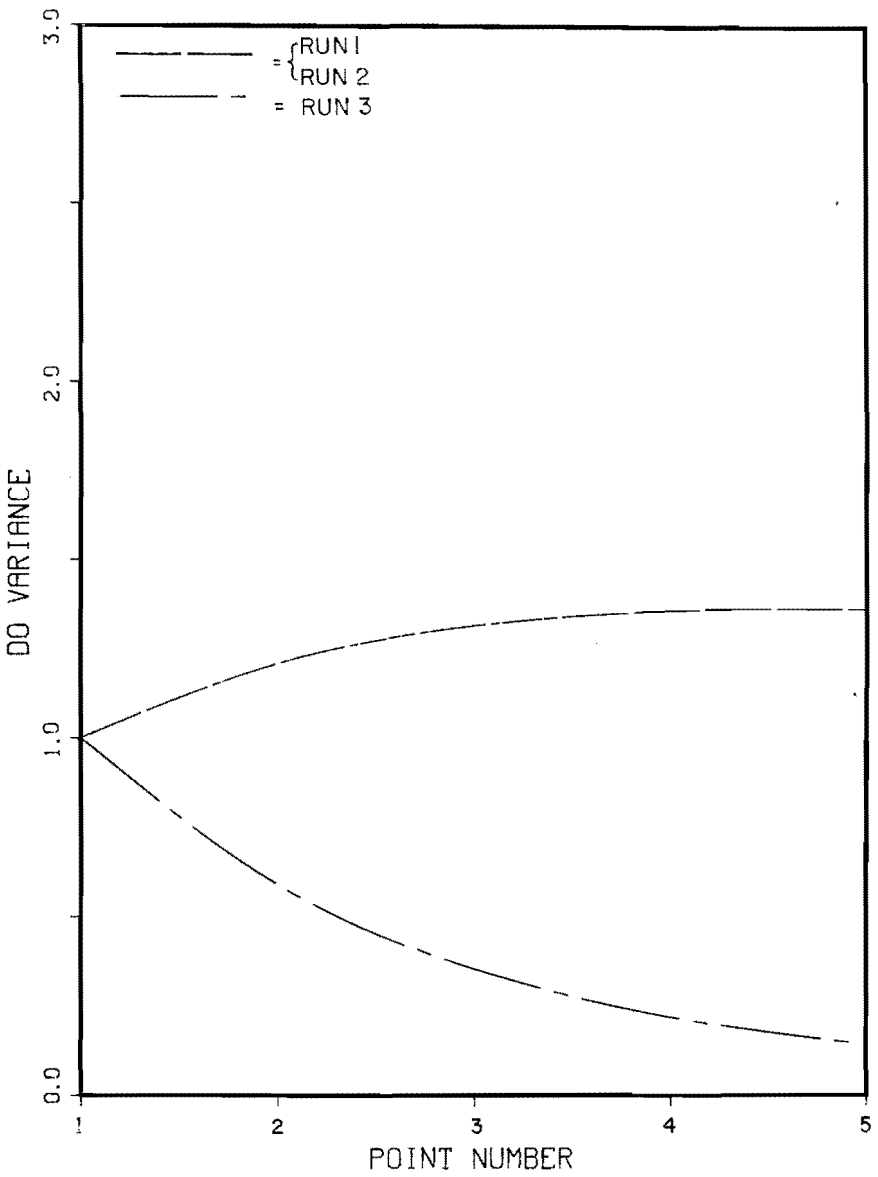


Figure 4.10. Variance of DO at points 1 through 5 for runs 1 through 3.

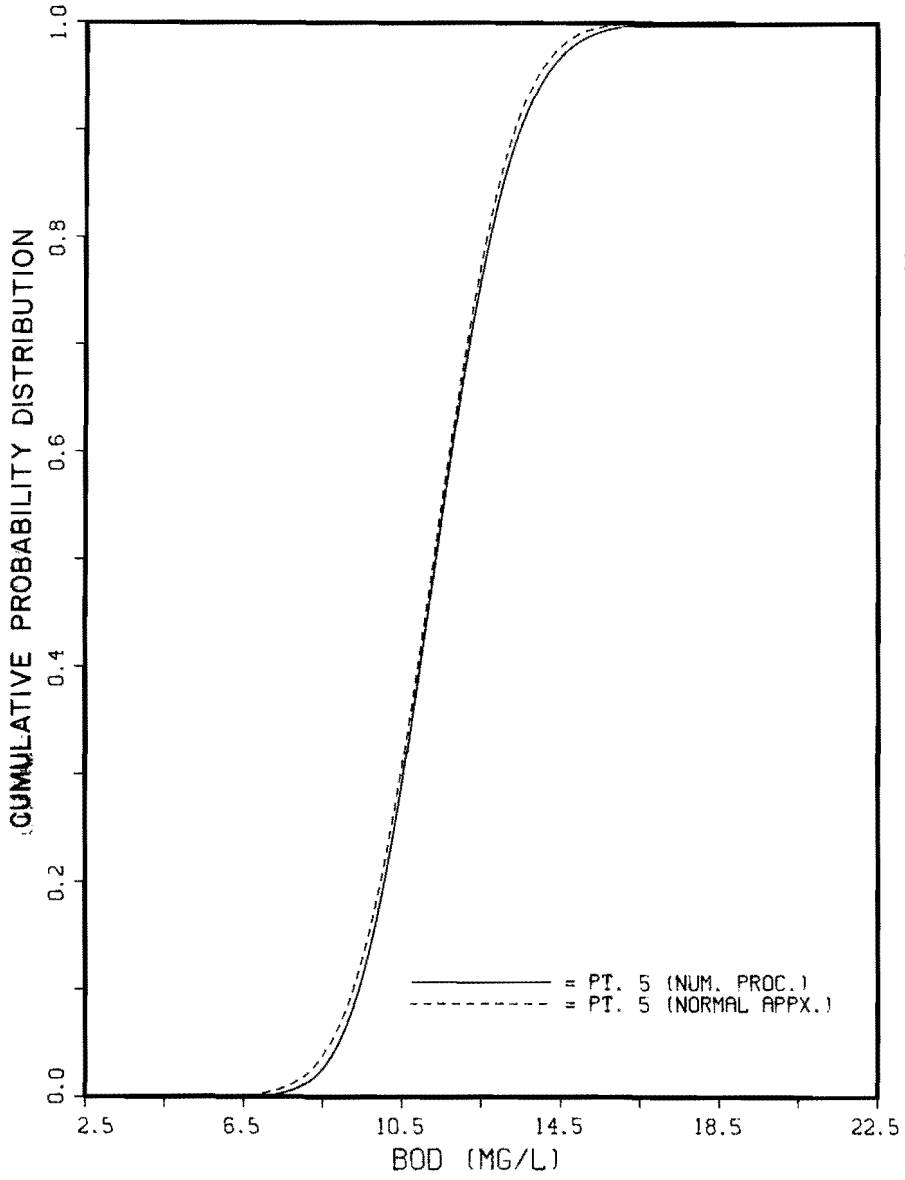


Figure 4.11. Comparison of the marginal cdf of BOD with a normal approximation at point 5 for run 2.

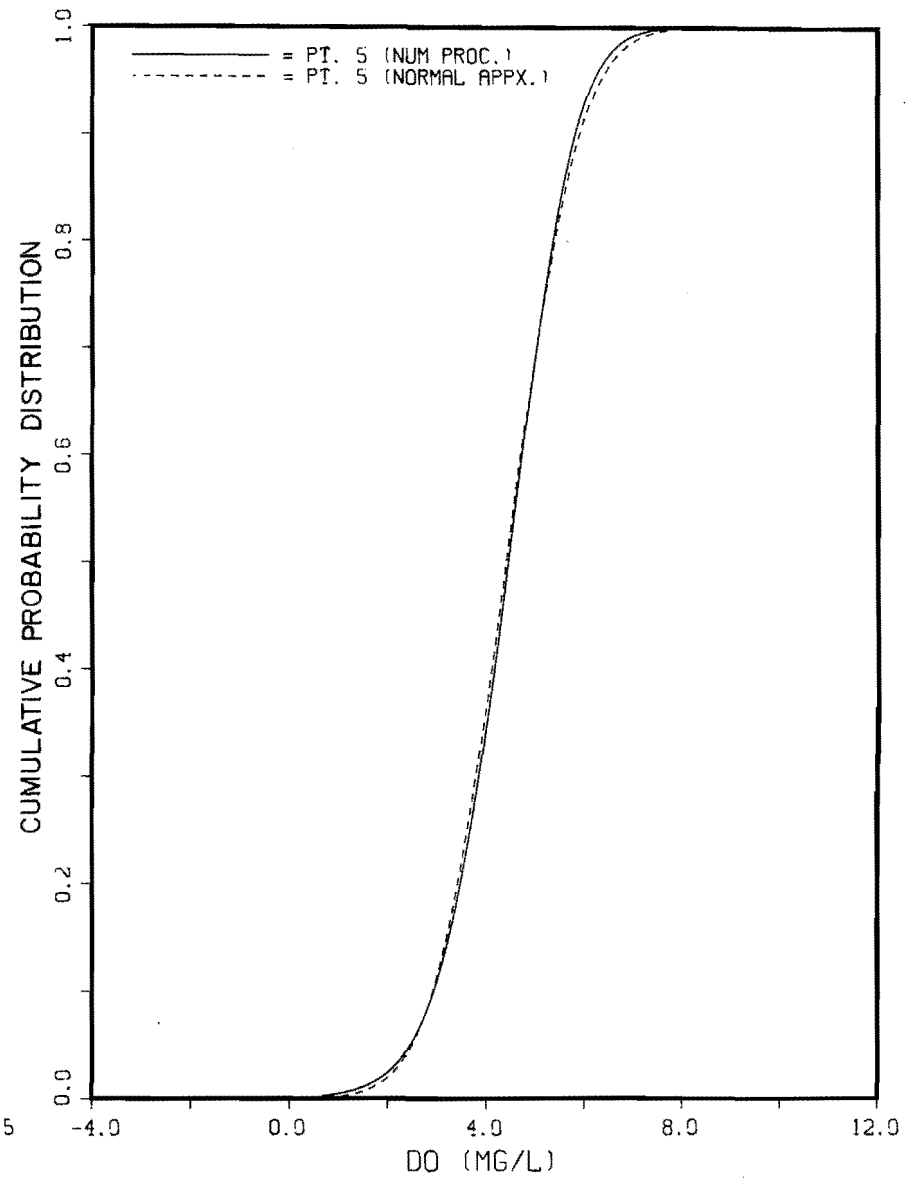


Figure 4.12. Comparison of the marginal cdf of DO with a normal approximation at point 5 for run 2.

BOD concentration being less than or equal to 10.5 mg/ℓ is approximately 0.33, using only the cdf as determined by the Fokker-Plank equation, and 0.35 using cdf from the normal approximation. For all three runs the error that would result from using a normal approximation for the marginal cdf of BOD or DO is small. This is not surprising in the case of run 3 since *Soong* [1973] shows that the solution for an n-dimensional system of Ito differential equations with random inputs and Dirac delta or Gaussian initial condition will be an n-dimensional Gaussian distribution. It is surprising, however, that the marginal pdf of BOD and DO for run 2 is well approximated by a normal distribution. *Windham* [personal communication, 1979] has shown that with a Dirac delta initial condition, coefficient noise and deterministic inputs, the solution of the system of equations used in PSSAM will describe a lognormal distribution for BOD and a translated lognormal distribution for DO. Therefore, it would be reasonable to expect the marginal pdf of BOD and DO for run 2 to have positive skew. However, the marginal cdf's of BOD and DO for run 2 are not visibly skewed. First, the normal initial condition dampens the skew produced by the coefficient noise. Second, the coefficient of skew expected for sensitivity run 2 is so small that even if BOD and DO had a lognormal distribution, the cdf would appear symmetric. The coefficient of skew (CS) for the lognormal distribution is given by the following equation:

$$CS = 3C_V + C_V^3 \qquad (4.1)$$

in which C_V is the coefficient of variation (standard deviation divided by the mean). For run 2 at point 5, the coefficients of variation for BOD and DO are 0.14 and 0.26, respectively, so the coefficients of skew for BOD and DO are 0.42 and 0.80, respectively. The asymmetry of a lognormal distribution with a CS = 0.80 is very small.

As previously shown, when using a normally distributed initial condition, the cdf of BOD and DO obtained from PSSAM is closely approximated by a normal distribution having the same mean and variance as BOD and DO. This suggests that instead of solving the Fokker-Plank equation to obtain the pdf of BOD and DO, it would be computationally easier and faster to solve the moment equations for the mean vector and covariance matrix and approximate the marginal pdf and cdf of BOD and DO using a normal distribution.

To investigate how well the marginal cdf of BOD and DO could be approximated with a normal distribution when a non-normal initial condition is used, run 2 was repeated. The initial condition of BOD was arbitrarily assumed to have an extreme value type I (for minimums) distribution. This distribution has a constant coefficient of skew equal to -1.1396. Although there is no physical justification for this precise value of the coefficient of skew for BOD, a negative coefficient of skew would be expected due to the first order decay of BOD (see Equation 3.19) which results in a greater probability of lower values of BOD than higher values. DO was arbitrarily assumed to have a lognormal initial condition. The standard deviation of DO at the headwater was increased to 5 mg/ℓ to give an initial coefficient of skew equal to 4.0. A positive coefficient of skew for DO is justified by the first order decay of BOD and first order reaeration both of which result in a greater probability of higher values of DO than lower values. The distributions of BOD and DO at the headwater must be assumed to be independent. The marginal pdf of BOD and DO at points 1 through 5 is shown in Figures 4.13 and 4.14, respectively. As the distance from the headwater increases, the skew of the pdf for both BOD and DO appears to decrease.

The marginal cdf's of BOD and DO at points 1, 3, and 5, are compared in Figures 4.15 through 4.20 with that of a normal distribution with the same mean and variance. The skew of the BOD distribution is small enough so that even at the headwater (point 1) the cdf is well approximated by the normal distribution (Figure 4.15). At points 3 and 5 the marginal cdf of BOD is almost identical to the normal approximation (Figures 4.17 and 4.19). The skew in the distribution of DO is large enough so that at the headwater the marginal cdf is approximated poorly by the normal cdf (Figure 4.16). The normal approximation improves as the distance from the headwater increases and is quite good at point 3 (Figure 4.18) and point 5 (Figure 4.20).

The results from the sensitivity runs indicate that it may be possible to reduce the computational effort necessary to determine the marginal pdf and cdf of BOD and DO by using a normal approximation. The normal approximation method is not only computationally faster and easier, but it would allow the use of a greater number of state variables. The computational effort necessary to solve the moment equations for a 10-dimensional system is likely to be less than that required to solve the Fokker-Plank equation for the joint pdf of two state variables. Further research is necessary to develop a better understanding of the tradeoffs.

It is also possible to write a system of equations for the third moments of the state variables and, therefore, compute the coefficient of skew. Further research is needed to define the upper value for the coefficient of skew for which the normal approximation of the cdf can be considered adequate for a particular application with a known loss function associated with errors in probability estimates.

Determination of whether the normal approximation is adequate would depend on the objectives of a particular model application. If the aquatic system can tolerate moderate changes in the water quality constituents being modeled without environmental or economic damage resulting, a relatively large error in the normal approximation may be acceptable. However, if the model is being used to estimate the pdf's of water quality constituents that are at or near some critical concentration, only a small error in the normal approximation would be acceptable. For example, many freshwater fish cannot tolerate a DO concentration less than 5.0 mg/ℓ. If the model were being used to estimate the pdf of DO in a blue ribbon trout stream, it would be important that error in the normal approximation be very small. In some cases where very limited funds are available, the approximation may be the only practical solution method. Then the tradeoff would

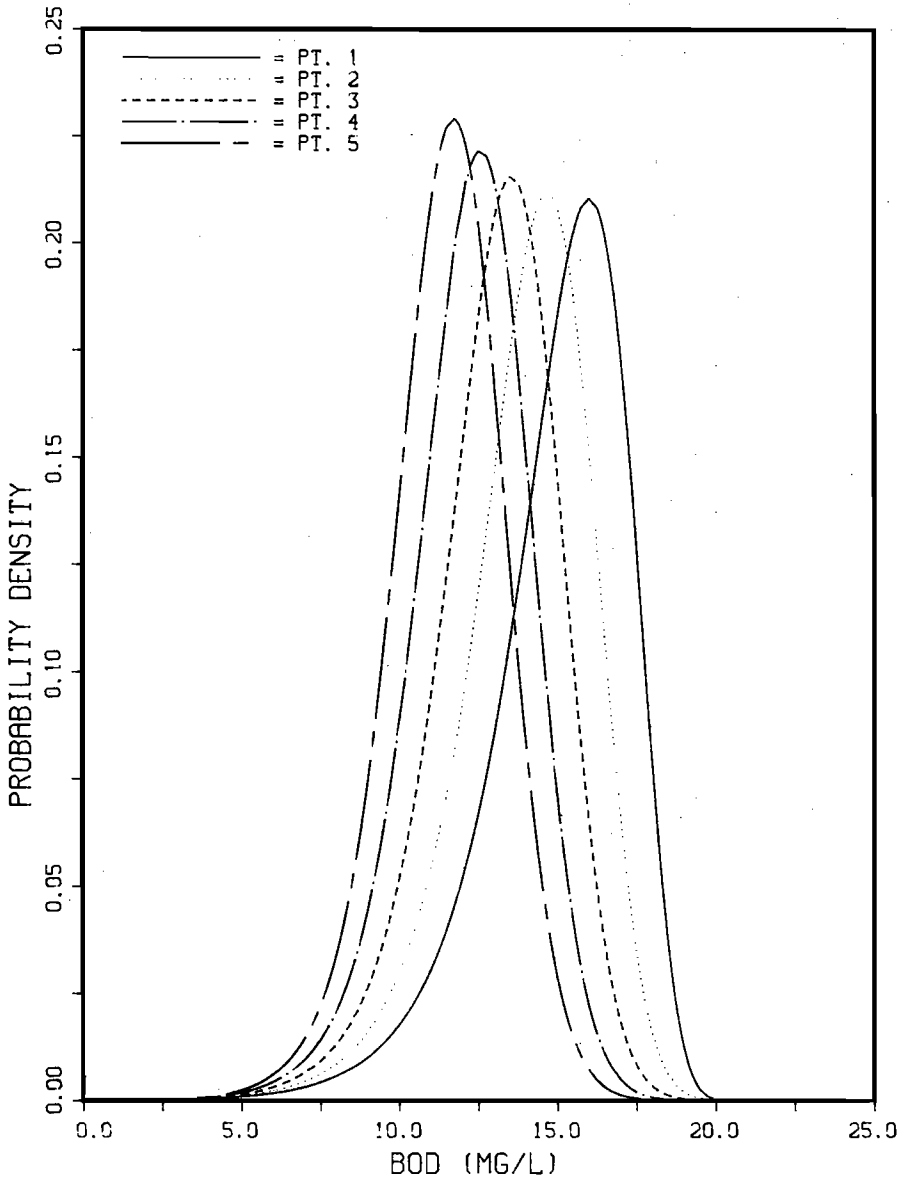


Figure 4.13. Marginal pdf of BOD at points 1 through 5 for run 2 with non-normal initial conditions.

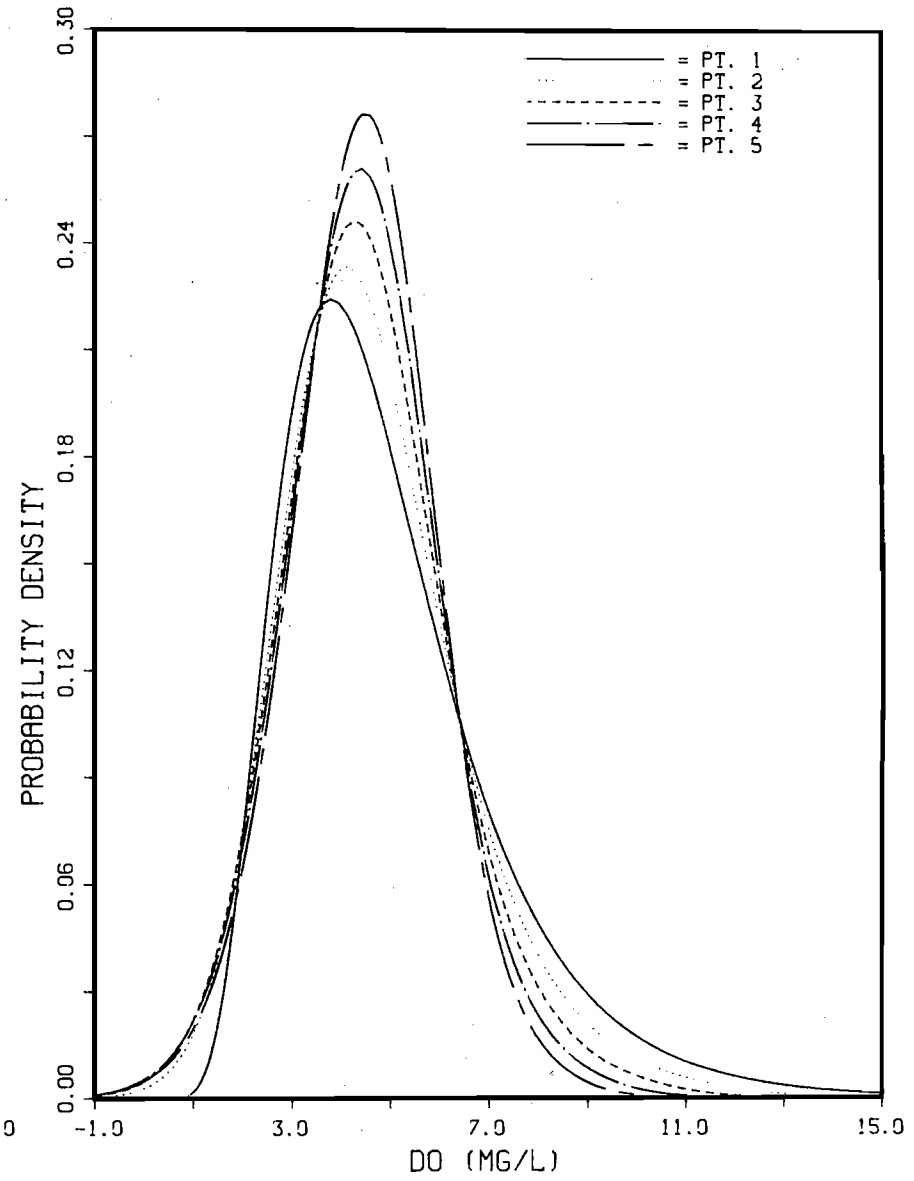


Figure 4.14. Marginal pdf of DO at points 1 through 5 for run 2 with non-normal initial conditions.

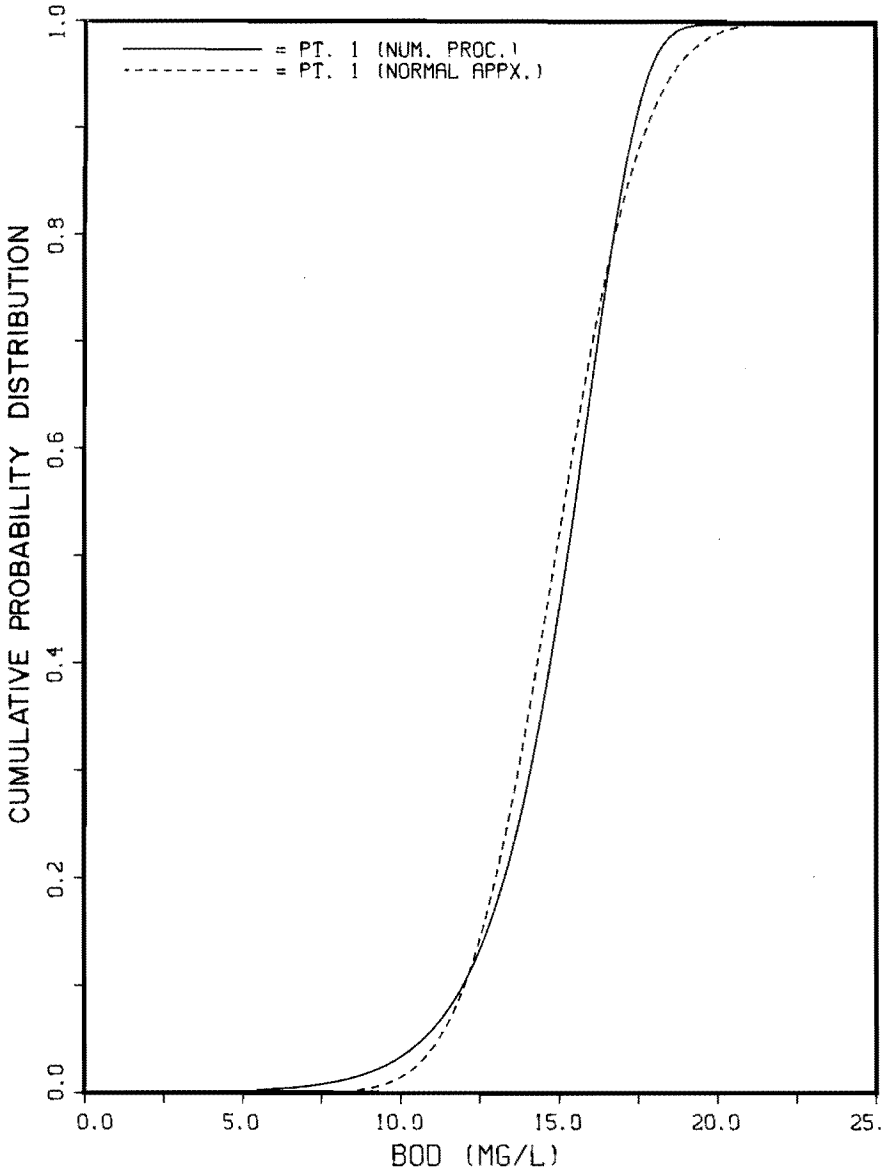


Figure 4.15. Comparison of the marginal cdf of BOD with a normal approximation at point 1 for run 2 with non-normal initial conditions.

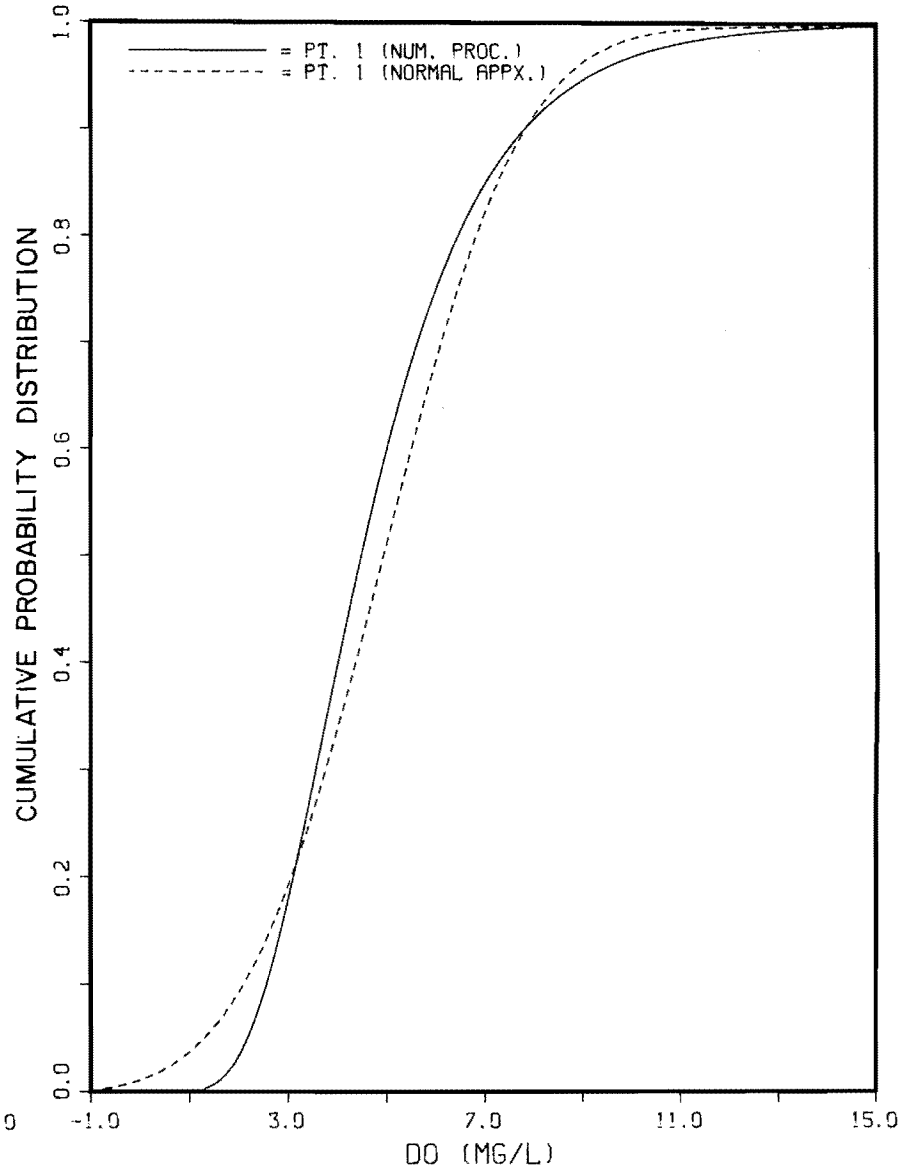


Figure 4.16. Comparison of the marginal cdf of DO with a normal approximation at point 1 for run 2 with non-normal initial conditions.

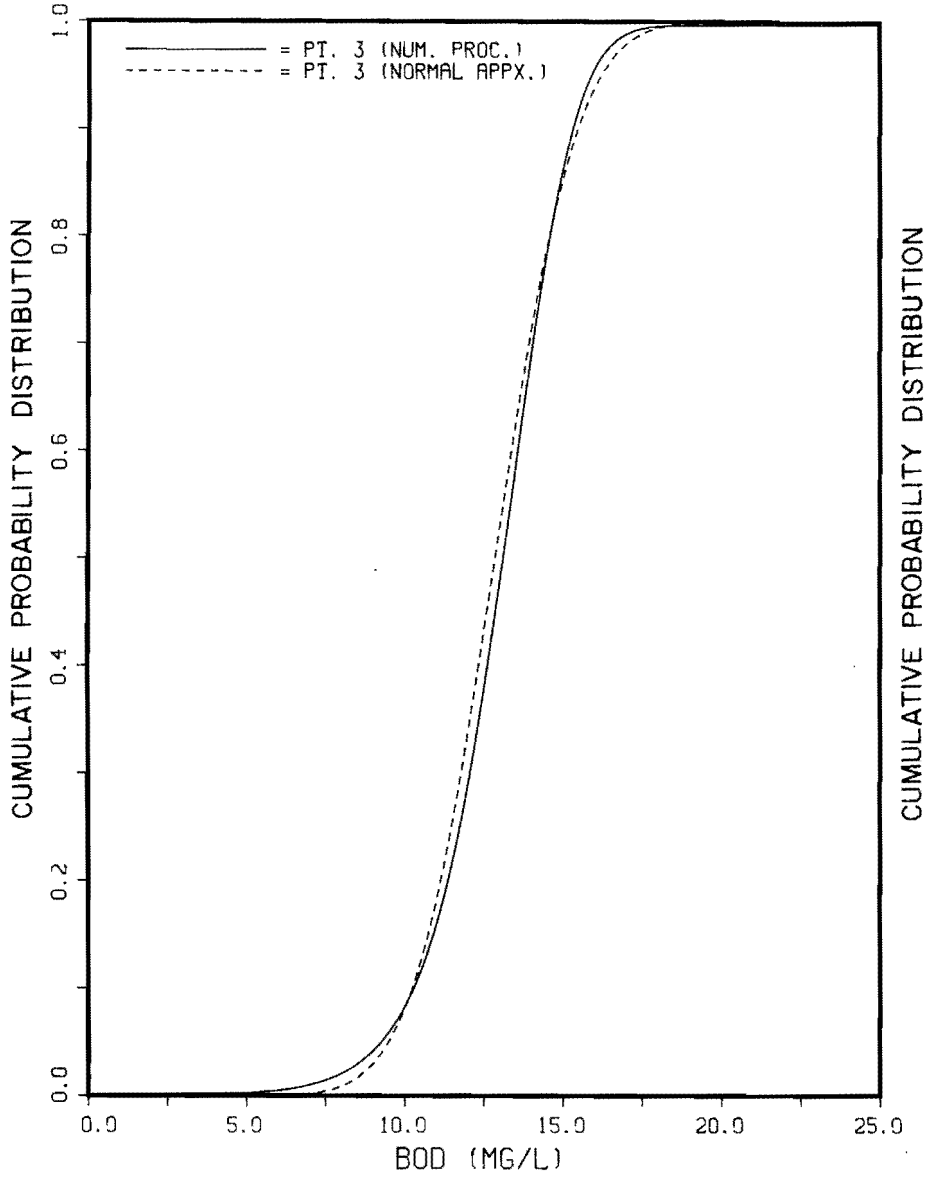


Figure 4.17. Comparison of the marginal cdf of BOD with a normal approximation at point 3 for run 2 with non-normal initial conditions.

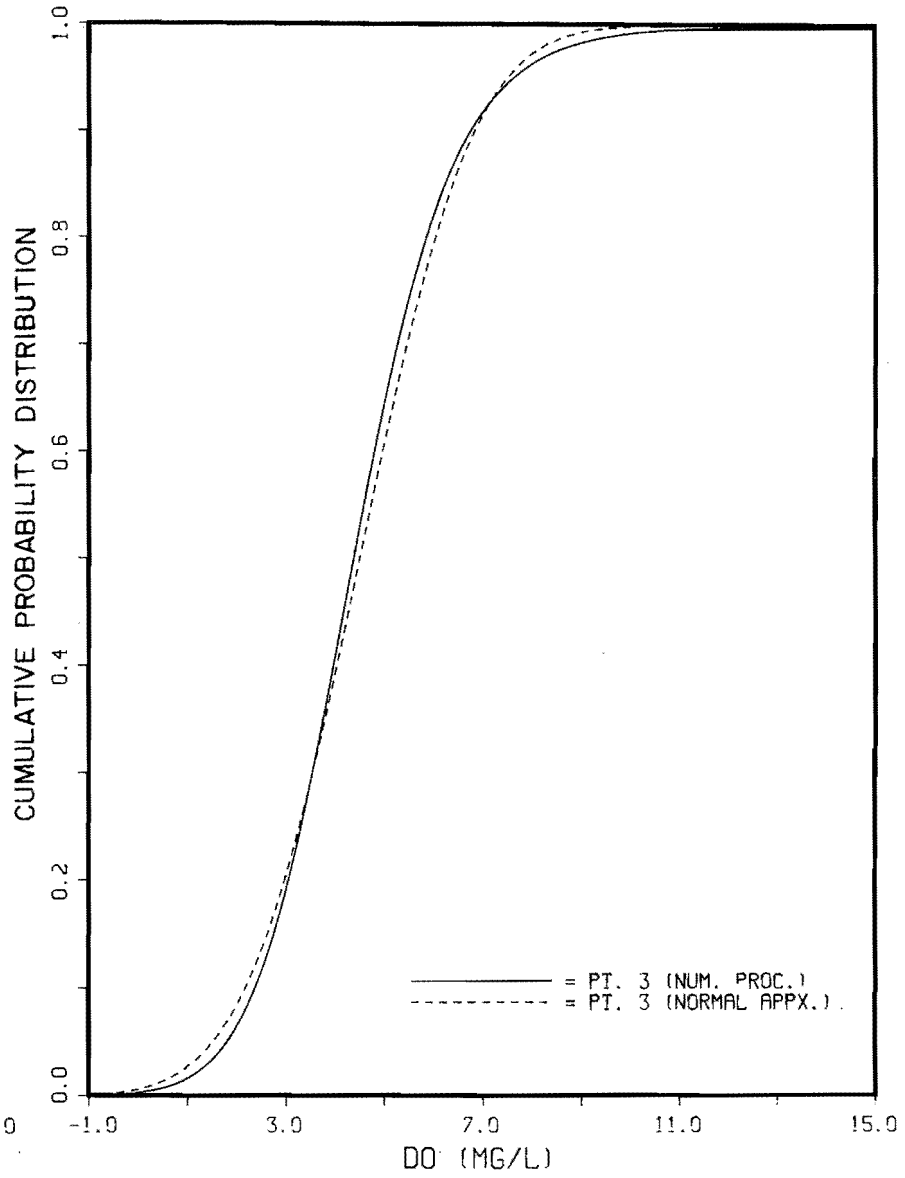


Figure 4.18. Comparison of the marginal cdf of DO with a normal approximation at point 3 for run 2 with non-normal initial conditions.

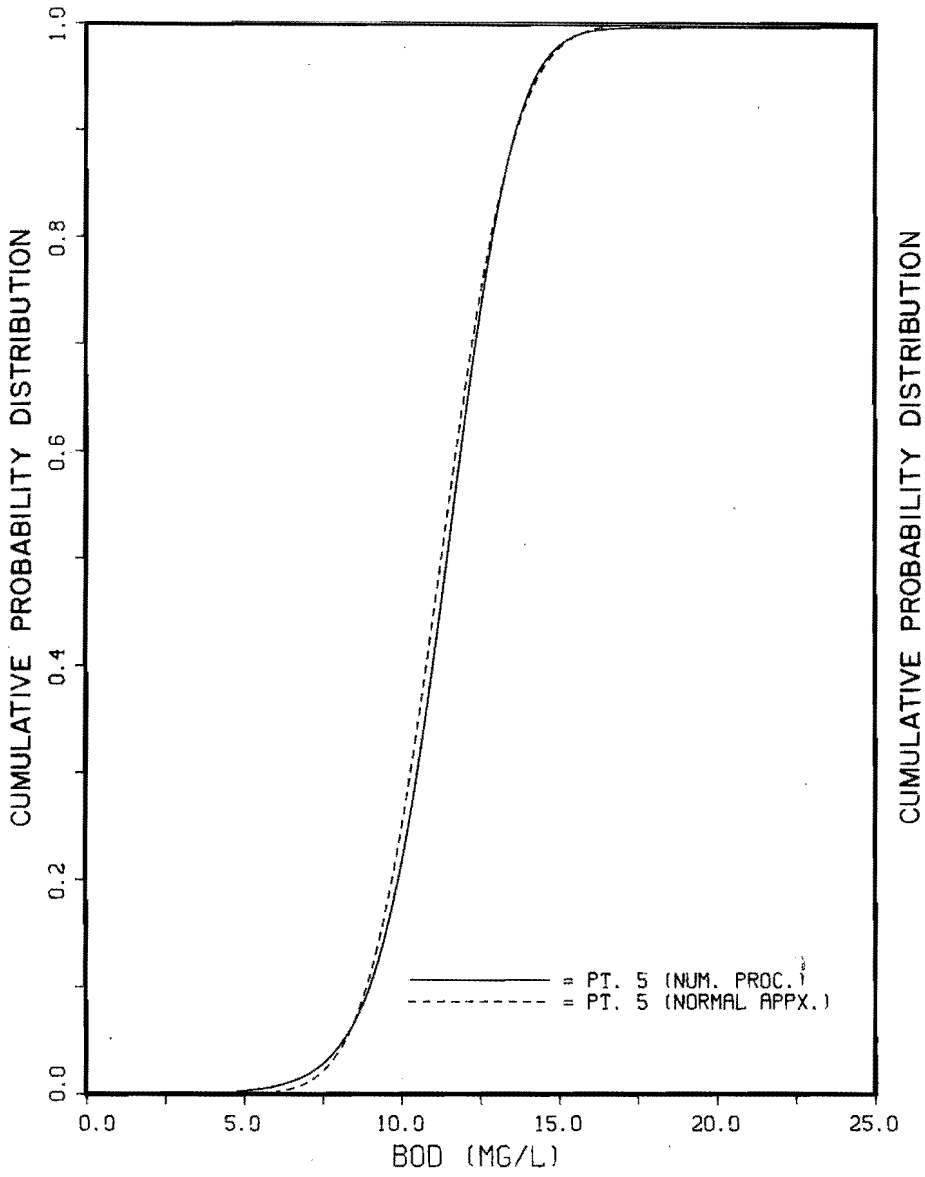


Figure 4.19. Comparison of the marginal cdf of BOD with a normal approximation at point 5 for run 2 with non-normal initial conditions.

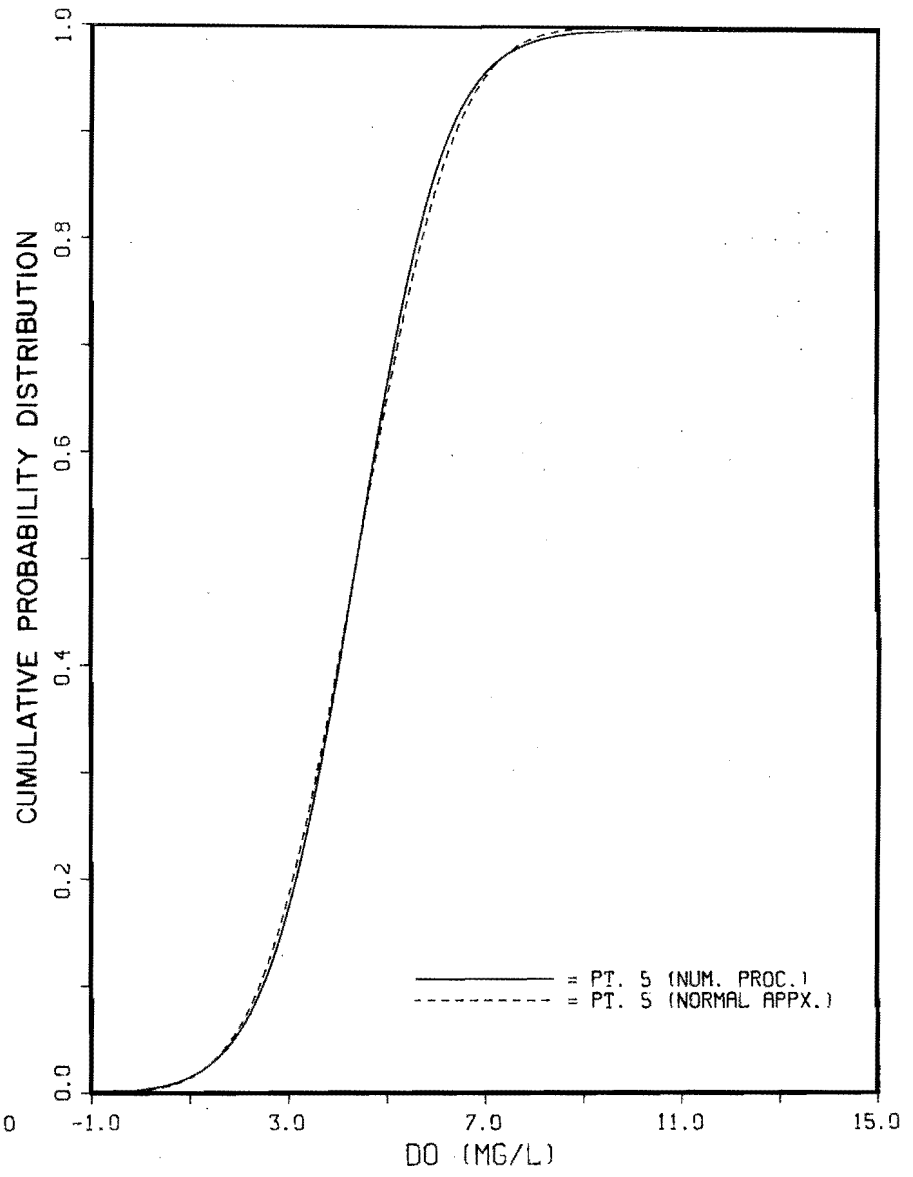


Figure 4.20. Comparison of the marginal cdf of DO with a normal approximation at point 5 for run 2 with non-normal initial conditions.

be between the normal approximation and deterministic modeling.

Two steps were taken to evaluate the accuracy of the numerical solution technique used to solve the Fokker-Plank equation for the joint pdf of BOD and DO. First, the mean and variance of BOD and DO were computed by numerically integrating the respective marginal pdf. Then they were compared with the mean and variance computed from the moment equations. Although the moment equations are solved numerically, a minimal number of computations is required and the numerical error should be very small. A comparison of the mean vector and covariance matrix of BOD and DO calculated by the marginal pdf's and the moment equations is shown in Table 4.4. In all sensitivity runs, the numerical difference between the mean and variance computed from the moment equations was less than or equal to 0.1. A typical comparison is given in Figure 4.21 where the marginal cdf of a normal distribution using the mean and variance computed from the two methods is shown for BOD at point 5 for run 1.

The numerical solution technique for the Fokker-Plank equation was also evaluated by comparing the joint pdf and cdf of BOD and DO computed in run 3 to the pdf and cdf of a normal distribution with the same mean and variance. As noted earlier, the distribution of BOD and DO should be normal since the coefficient noise was zero in run 3. Indeed, the computed marginal pdf and cdf of BOD and DO are nearly identical to the normal pdf and cdf for run 3. On the basis of the sensitivity runs, it can be concluded that the numerical solution technique used to solve the Fokker-Plank equation worked extremely well. Additional research may develop a solution algorithm which would allow the inclusion of more than two state variables.

Hypothetical Problem

In order to further explore the capabilities of PSSAM, it was applied to a more complex hypothetical problem. In particular, the error characteristics of the numerical quadrature algorithm used to determine the joint pdf of BOD and DO immediately downstream of a point load were evaluated.

Problem description

Figure 4.22 is a diagram of the river system used in the hypothetical problem. It consists of a headwater, three reaches, one point diversion, two point loads, and two check points. Tables 4.5 through 4.7 provide the necessary input data for the hypothetical problem. A summary of the river system layout and hydraulics is given in Table 4.5. A characterization of the water quality of the headwater and point loads is given in Table 4.6. The water quality equation coefficients and inputs are given in Table 4.7. The input and coefficient noise standard deviation parameters were assumed to be 20 and 40 percent, respectively, corresponding to the values used in sensitivity run 1.

Table 4.4. Comparison of the mean vector and covariance matrix calculated by the numerical procedure and the moment equations.

		BOD				DO				BOD-DO Covariance	
		Numerical Procedure		Moment Equations		Numerical Procedure		Moment Equations		Numerical Procedure	Moment Equations
Run	Point	Mean (mg/ℓ)	Variance $(mg/ℓ)^2$	Mean (mg/ℓ)	Variance $(mg/ℓ)^2$	Mean (mg/ℓ)	Variance $(mg/ℓ)^2$	Mean (mg/ℓ)	Variance $(mg/ℓ)^2$	$(mg/ℓ)^2$	$(mg/ℓ)^2$
1	1	15.0	3.0	15.0	3.0	5.0	1.0	5.0	1.0	1.0	1.0
	2	13.9	2.9	13.9	2.9	4.7	1.2	4.7	1.2	1.0	1.0
	3	13.0	2.8	13.0	2.8	4.6	1.3	4.6	1.3	1.0	1.0
	4	12.2	2.6	12.1	2.6	4.5	1.3	4.5	1.3	0.9	0.9
	5	11.5	2.5	11.4	2.5	4.5	1.3	4.5	1.4	0.8	0.8
2	1	15.0	3.0	15.0	3.0	5.0	1.0	5.0	1.0	1.0	1.0
	2	13.9	2.9	13.9	2.9	4.7	1.2	4.7	1.2	1.0	1.0
	3	13.0	2.8	13.0	2.8	4.6	1.3	4.6	1.3	1.0	1.0
	4	12.2	2.6	12.1	2.6	4.5	1.3	4.5	1.3	0.9	0.9
	5	11.5	2.5	11.4	2.5	4.5	1.3	4.5	1.4	0.8	0.8
3	1	15.0	3.0	15.0	3.0	5.0	1.0	5.0	1.0	1.0	1.0
	2	14.0	2.5	14.0	2.5	4.7	0.6	4.7	0.6	0.6	0.6
	3	13.0	2.0	13.0	2.0	4.6	0.4	4.6	0.4	0.4	0.3
	4	12.2	1.7	12.1	1.7	4.5	0.2	4.5	0.2	0.2	0.2
	5	11.5	1.4	11.4	1.4	4.5	0.1	4.5	0.1	0.1	0.1

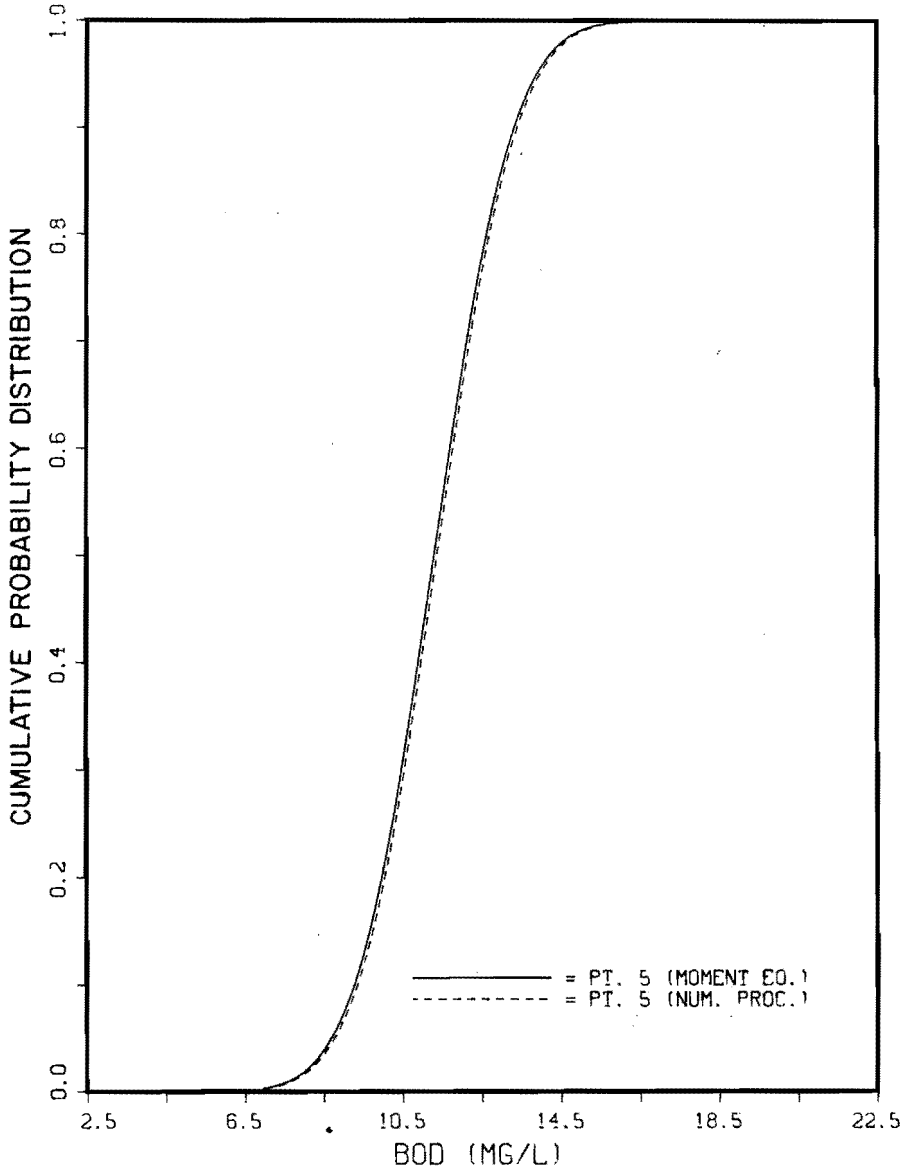


Figure 4.21. Comparison of the normal cdf at point 5 for run 1 with the mean and variance calculated by the moment equations and the marginal cdf of BOD.

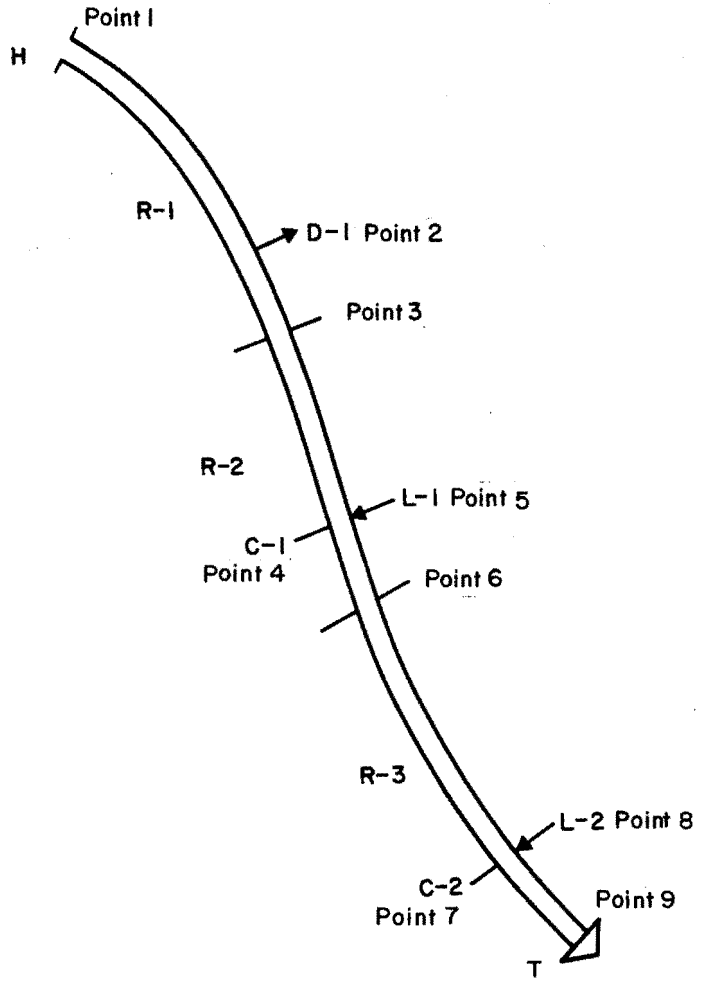


Figure 4.22. River system layout for hypothetical problem.

Table 4.5. River system layout and hydraulics for hypothetical problem.

Point Number	Description	Location (km)	Input Flow (m^3/sec)	Lateral Inflow for Reach		River Flow (m^3/sec)	Ave. Reach Vel. (m/sec)	Ave. Reach H. Rad. (m)
				Surface (m^3/sec/km)	Ground (m^3/sec/km)			
1	Head of Reach 1 (Headwater)	30.	5.0	0.02	0.0	5.00	0.25	1.32
2	Point Diversion	23.	-0.5			4.64		
3	Head of Reach 2	20.		0.02	0.01	4.70	0.25	1.22
4	Check Point 1	15.				4.85		
5	Point Load 1	15.	0.2			5.05		
6	Head of Reach 3	12.		0.01	0.03	5.14	0.30	1.28
7	Check Point 2	4.				5.46		
8	Point Load 2	4.	0.3			5.76		
9	Termination	0				5.92		

Table 4.6. Headwater and point load water quality characterization.

Description	BOD		DO		BOD-DO Covariance $(mg/\ell)^2$
	Mean (mg/ℓ)	Standard Deviation (mg/ℓ)	Mean (mg/ℓ)	Standard Deviation (mg/ℓ)	
Headwater	15.0	3.00	6.00	1.44	3.09
Point Load 2	20.0	16.0	3.00	0.36	2.08
Point Load 2	25.0	25.0	2.00	0.16	1.73

Table 4.7. Inputs, water temperature and water quality coefficients for hypothetical problem.

Constituent	Symbol	Units	Description	Coefficient Use for Reach 1	2	3
BOD	$\beta_{1,1}$	1/day	First-order decay rate	0.26	0.32	0.33[1]
	$\beta_{1,2}$	1/day	First-order removal rate	0.0	0.0	0.0
	L_1	$g/m^2/day$	Leach rate	0.10	0.10	0.15
	X_{S_1}	mg/ℓ	Lateral surface inflow	15.0	10.0	10.1
	X_{G_1}	mg/ℓ	Lateral subsurface inflow	5.0	8.0	8.0
DO	$\beta_{2,1}$	1/day	Reaeration rate	3.21	3.66	3.32[1]
	$\beta_{2,2}$	km	Elevation	1.15	1.1	1.05
	$\beta_{2,3}$	mg/ℓ/day	Net oxygen production by phytoplankton	1.00	1.20	1.20
	$\beta_{2,4}$	$(g/m^2/day)/(mgO_2/ℓ)$	Benthic uptake of oxygen	0.20	0.30	0.35
	L_2	$g/m^2/day$	Leach rate	0.0	0.0	0.0
	X_{S_2}	mg/ℓ	Lateral surface inflow	3.0	2.0	2.0
	X_{G_2}	mg/ℓ	Lateral subsurface inflow	0.0	0.0	0.0
Temperature	T	°C	Water temperature	17.0	18.0	19.0

[1] Coefficient value is corrected to 20°C.

Results from hypothetical problem

No numerical stability problems were encountered in using PSSAM to solve Equation 3.66 while running the hypothetical problem. The normal approximation to the marginal cdf of BOD and DO was found to be just as good for the hypothetical problem as for the sensitivity problem.

The 15 point Gauss-Legendre quadrature algorithm used to determine the joint pdf of BOD and DO immediately downstream of a point load was evaluated by computing the volume under the joint pdf. The volume under any joint pdf should always be equal to 1.0. The deviation of the volume of the joint pdf immediately downstream of both point loads was within a few hundredths of 1.0 indicating the quadrature algorithm performed reasonably well (see Table 4.8).

Computational Aspects

All model runs were made on the Burroughs 6700 computer located on the Utah State University campus. Each sensitivity run required 11 minutes of central processor time with a total cost of $14. The hypothetical problem required 40 minutes of central processor time with a total cost of $65. The difference in the computational time for the two problems was due to the longer stream length being simulated and the necessity of calculating the joint pdf of BOD and DO immediately below the two point loads in the hypothetical problem. The processor times may seem high but it would be noted that the Burroughs 6700 computer is an extremely slow machine. The IBM 360 series computer, the CDC 6400 series computer, and the Univac 1108 computer all are approximately 10 times faster than the Burroughs 6700.

Table 4.8. Volume under joint probability density function of BOD and DO upstream and downstream of point loads.

Point Number	Location	Volume under joint pdf
4	Immediately upstream of point load 1	1.06
5	Immediately downstream of point load 1	1.03
7	Immediately upstream of point load 2	1.06
8	Immediately downstream of point load 2	1.07

CHAPTER V

SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

Summary

A random differential equation has been derived and a solution algorithm has been written into a computer program that provides a probabilistic river water quality model with the capability of determining the joint and marginal probability density functions of BOD and DO at any point in a river. The one dimensional steady-state model can be applied to a river system with any reasonable number of point loads and diversions and patterns of lateral surface and subsurface inflow. The model can simultaneously consider randomness in the initial conditions, inputs, and coefficients of the water quality equations. Any empirical or known distribution can be used for the initial condition. The randomness in the water quality equation inputs and coefficients were modeled as Gaussian white noise processes. The joint pdf of BOD and DO was determined by numerically solving the Fokker-Plank equation. Moment equations were developed which allowed the mean and variance of the marginal distributions of BOD and DO to be calculated independently of the joint pdf. An upper limit on the coefficient noise standard deviation parameter was presented for which the BOD-DO covariance matrix will be asymptotically stable.

The probabilistic river water quality model was applied to two problems, a sensitivity problem and a hypothetical problem. The sensitivity problem, which consisted of a headwater and four check points, was used to gain familiarity with the simulation model and determine the sensitivity of the model responses to changes in the standard deviation parameter of the input and coefficient noise. The standard deviation parameter of the input noise was varied between zero and 30 percent of the respective input, while the coefficient noise standard deviation parameter was varied between zero and 50 percent of the respective coefficient. The model responses were found to be fairly sensitive to changes in the coefficient noise standard deviation parameter but relatively insensitive to changes in the input noise standard deviation parameter. The possibility of using the moment equations and a normal approximation in lieu of calculating the joint pdf of BOD and DO was discussed and the results were found to be similar to the model results. The accuracy of the numerical solution technique for the Fokker-Plank equation was also discussed.

The hypothetical problem was used to evaluate the performance of the model in simulating a more complex river system. The hypothetical problem was used to evaluate the numerical quadrature algorithm used to determine the joint pdf of BOD and DO immediately downstream of a point load. The problem consisted of a headwater, three reaches, one point diversion, and two point loads and check points. The numerical solution technique used to determine the joint pdf of BOD and DO was stable throughout the simulation. The quadrature algorithm was judged to have performed adequately for both the point loads based on the error in the volume under the joint pdf.

Conclusions

The following conclusions have been developed from results and experience gained during this study. Each conclusion is conditional on the limitations made in the model development and summarized at the end of Chapter III.

1. Representing the randomness in the water quality equation inputs and coefficients as a Gaussian white noise process is appealing since techniques are available to solve the resulting random differential equations for the pdf of the state variable and because the mean of the random process is the deterministic solution.

2. The randomness in the coefficients in the water quality equations appears to have a significantly greater influence on the total model prediction uncertainty than does the randomness in the equation inputs. In the sensitivity problem, the input randomness contribution to the prediction uncertainty was negligible. However, this conclusion would not be expected to hold for unsteady conditions.

3. The normal approximation of the marginal pdf of BOD and DO was good for both the sensitivity and hypothetical problems, but judgments as to the adequacy of this approximation depend on the use to which the pdf is to be put and the loss function associated with errors in probability estimates. Using the moment equations to calculate the mean and variance of the distribution and then approximating the pdf and cdf with a normal distribution is computationally easier and faster (approximately 10 times faster in the sensitivity problem) than solving the Fokker-Plank equation for the joint pdf.

4. Based on the results and the wide range in input and coefficient noises treated in the sensitivity runs, it appears that it would usually be advantageous to approximate the marginal pdf and cdf of BOD and DO with a normal distribution. If the initial condition is normally distributed and the coefficient noise is zero, the normal approximation is exact. Even if the initial conditions are not normal, and the coefficient noise is non-zero, the normal approximation may be adequate.

5. Computational costs and solution results indicate that the probabilistic river water quality model developed herein could be a viable tool in river basin water quality management. Computational costs for the reasonably complex hypothetical problem were only $65. That cost could be cut significantly by using a normal approximation of the pdf and cdf of BOD and DO.

Recommendations

The following recommendations for further work are based on experience gained during this study:

1. Initiate a river water quality data collection program to measure river water quality characteristics on streams from a wide range of flows, pollution loadings, and other characteristics. Ideally, continuous data on pertinent physiochemical characteristics (flow rate, temperature, water depth, nutrient concentrations, etc.) would be collected at several sampling points for at least one year. This would provide the information necessary to estimate the water quality input and verify the model under a wide range of conditions.

2. Make a determination of the relative importance of water quality equation input and coefficient randomness to the overall model prediction uncertainty for a wide variety of river systems.

3. Determine whether a normal approximation to the marginal pdf of BOD and DO would be adequate for a wide range of initial conditions, coefficients, and inputs for the water quality equations. If the approximation is nearly always adequate, the model could be simplified by solving the moment equations and using a normal approximation to the distribution of BOD and DO.

4. Investigate the use of an upper bound on the coefficient of skew for which a normal approximation to the marginal pdf of BOD and DO is adequate.

5. Consider the possibility of adding or using different state variables. The former may prove to be impossible if the Fokker-Plank equation must be numerically solved to determine the joint pdf of the state variables. However, if the normal approximation to the pdf of the state variables is used, then all that would be necessary is to develop first and second moment equations for the larger state vector.

6. Modify the model so that it will simulate the dynamic nature of rivers.

7. Interface a general economic model with the probabilistic river water quality model. Some features of the economic model might include an algorithm to calculate environmental damage functions based on the probabilistic nature of pollution discharge to the river and the probabilistic nature of the pollutant concentration in the river. The combined models could then be used as a regional planning and control model that would minimize the cost of wastewater treatment in a river basin subject to environmental damage constraints. A problem that would need to be addressed is how to handle randomness in economic damage functions which is probably greater than that in the water quality model.

8. Investigate whether the assumption of mutually independent noise processes for the model inputs and coefficients introduces a significant error in the model predictions of the noise processes are correlated.

9. Determine, for the given deterministic model structure, the optimal combination of deterministic and random variables which maximizes the amount of the prediction uncertainty which is represented under the constraint of not being able to treat random variables which appear in multiplicative terms in the equations.

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APPENDIX

Derivation of Joint pdf of BOD and DO Downstream of a Point Load

From Equations 3.45 and 3.46 we have the following expressions for X_1 and X_2:

$$X_1 = \alpha X_{1_u} + \alpha X_{1_\ell} \tag{A.1}$$

$$X_2 = \alpha X_{2_u} + \alpha X_{2_\ell} \tag{A.2}$$

If two dummy random variables X_3 and X_4 are defined as follows:

$$X_3 = X_{1_\ell} \tag{A.3}$$

$$X_4 = X_{2_\ell} \tag{A.4}$$

then the joint pdf of (X_1, X_2, X_3, X_4) is

$$f_{\underline{X}}(x_1 x_2 x_3 x_4) = f_{X_{1_u} X_{2_u} X_{1_\ell} X_{2_\ell}}(x_{1_u} x_{2_u} x_{1_\ell} x_{2_\ell}) |J| \tag{A.5}$$

where $f_{X_{1_u} X_{2_u} X_{1_\ell} X_{2_\ell}}$ is the joint pdf of $(X_{1_u} X_{2_u} X_{1_\ell} X_{2_\ell})$. The Jacobian, J, of the transformation is defined as follows:

$$J = \begin{vmatrix} \frac{\partial X_{1_u}}{\partial X_1} & \frac{\partial X_{1_u}}{\partial X_2} & \frac{\partial X_{1_u}}{\partial X_3} & \frac{\partial X_{1_u}}{\partial X_4} \\ \frac{\partial X_{2_u}}{\partial X_1} & \frac{\partial X_{2_u}}{\partial X_2} & \frac{\partial X_{2_u}}{\partial X_3} & \frac{\partial X_{2_u}}{\partial X_4} \\ \frac{\partial X_{1_\ell}}{\partial X_1} & \frac{\partial X_{1_\ell}}{\partial X_2} & \frac{\partial X_{1_\ell}}{\partial X_3} & \frac{\partial X_{1_\ell}}{\partial X_4} \\ \frac{\partial X_{2_\ell}}{\partial X_1} & \frac{\partial X_{2_\ell}}{\partial X_2} & \frac{\partial X_{2_\ell}}{\partial X_3} & \frac{\partial X_{2_\ell}}{\partial X_4} \end{vmatrix} \tag{A.6}$$

therefore

$$J = 1/\alpha^2 \tag{A.7}$$

If the upstream concentrations of BOD and DO (X_{1_u}, X_{2_u}) are independent of the concentrations of BOD and DO in the point load (X_{1_ℓ}, X_{2_ℓ}), then

$$f_{X_{1_u} X_{2_u} X_{1_\ell} X_{2_\ell}}(x_{1_u} x_{2_u} x_{1_\ell} x_{2_\ell}) = f_{X_{1_u} X_{2_u}}(x_{1_u} x_{2_u}) f_{X_{1_\ell} X_{2_\ell}}(x_{1_\ell} x_{2_\ell}) \tag{A.8}$$

$$f_{\underline{X}}(x_1 x_2 x_3 x_4) = (1/\alpha^2) f_{X_{1_u} X_{2_u}}(x_{1_u} x_{2_u}) f_{X_{1_\ell} X_{2_\ell}}(x_{1_\ell} x_{2_\ell}) \tag{A.9}$$

Integrating over the dummy variables X_3 and X_4 and making appropriate substitutions yields the joint pdf of downstream concentration of BOD and DO:

$$f_{X_1 X_2}(x_1 x_2) = \frac{1}{\alpha^2} \int_{X_{1_\ell}} \int_{X_{2_\ell}} f_{X_{1_u} X_{2_u}}\left(\frac{x_1 - \gamma x_{1_\ell}}{\alpha} \quad \frac{x_2 - \gamma x_{2_\ell}}{\alpha}\right) f_{X_{1_\ell} X_{2_\ell}}(x_{1_\ell} x_{2_\ell}) dX_{1_\ell} dX_{2_\ell} \tag{A.10}$$