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STOCHASTIC MODELLING OF WATER QUALITY DATA



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PREFACE

Water is one of the most essential constituents of the human environment. As a part of the general concern for environment, water quality become an important water resources issue due to the increasing trend of pollution sources e.g. rapid population growth, rapid industrial development, increasing mining and petroleum operations, and too much use of fertilizers and pesticides in agriculture.

Water quality is usually described by set of physical, chemical, and biological parameters which are mutually inter-related and vary according to a complex function of natural and man made interactions in both time and space. Both of these interaction mechanisms affecting water quality are to a certain extent affected by the laws of chance. This is particularly true for the effects introduced through variation in the natural hydrologic cycle. To properly interpret water quality data, it is critical that the random nature of water quality variables be appreciately understood. Emphasis should be made on understanding how water quality parameters evolve under natural and society affected conditions in various bodies of water. Furthermore, the deterministic water quality analysis is complicated by the fact that many of the factors which influence variations in water quality are not well defined. These factors may be further obscured by the occurrence of random events. Consequently, the application of stochastic techniques to water quality data has become necessary in order to generate the data for various water quality parameters which can be used for water quality modelling

studies. The present study gives a short review on stochastic modelling with particular emphasis on river water quality.

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ABSTRACT

In the past two decades, many mathematical water quality models have been developed to simulate physical, chemical, and biological processes occurring in river water. Their possible applications range from identifying in-streaming processes affecting river water quality to forecasting the quality for operational purposes.

It was a common practice to describe problems related to chemical and biological processes in river waters through deterministic differential equations. Since the deterministic model provides a single response for each set of model parameters and initial conditions, there is always some uncertainty, both in the evaluation of field data and in the use of mathematical models to predict the outcome of natural processes. The full representation of the process responses is usually too complicated and may be too costly to develop. Due to inherent variability and randomness in natural processes and their measurements, all these sources of uncertainty could be represented as input forcing terms in the balance equations. The initial conditions may be random, either because of the imperfect real initial conditions or because of the biased measurements. The model coefficients (rate constants) may be random due to variations in measurements.

Number of models have been proposed in recent years which treat water quality processes as stochastic. In the present study a review of the available literature on 'stochastic water quality modeling' have been made.

1.0 INTRODUCTION

Water quality management may be defined as the effort made by the society to control the physical, chemical and biological characteristics of water. Efforts dictate to control the impacts of society upon the quality of water. Water quality in the environment, however, is the result of two primary casual mechanisms: first the activities of society, and second the natural hydrologic cycle. Therefore, water quality management should deal with both events, infact it attempts to control only one-the activities of society. Both the mechanisms may be described as stochastic processes in that each, to some degree, is governed by the laws of chance. Thus, water quality, from a broad perspective, can be considered a random variable.

Water quality conditions over a large area are the function of complex natural and man-made causes and of the resulting interactions in both time and space. Both of these mechanisms controlling water quality are to a certain extent affected by the laws of chance. This is particularly true for the effects introduced through variation in the natural hydrologic cycle. To properly interpret water quality data, it is critical that the random nature of water quality variables be appreciately understood. Emphasis should be made on understanding how water quality properties evolve under natural and society affected conditions in various bodies of water.

Water quality is usually described by set of physical, biological and chemical variables which are mutually interrelated. Expressing some water quality variables in terms of other water

quantity variables is of continuous interest to water resources specialists. Also it is useful to describe water quality variables both in statistical terms, such as parameters of distributions, and in terms of various river basin characteristics.

Water quality analysis is complicated by the fact that many of the factors which influence variations in water quality are not well defined. These factors may be further obscured by the occurrence of random events. Consequently the application of statistical techniques of water quality data analysis has become necessary.

Water quality variables are classified herein as random variables, or more precisely as stochastic processes. Randomness means that the outcomes of observations of water quality variables are governed particularly by the laws of chance. Some aspects of outcomes are regular or predictable, such as the periodicity with day and year in some water quality variables, while the other parts of outcomes are governed by the laws of chance and cannot be predicted. The term stochastic process implies that one is interested in the value of the random variable as a function of time, space, or both. The variations in space and along time are partially or fully governed by the laws of chance.

Many variables are needed to completely describe the water quality processes. Several hundred variables have already been identified that may be of interest to different users in a comprehensive description of water quality processes. It is economically unfeasible to regularly record, observe or sample all these hundreds of quality variables. Therefore, it is necessary to establish a special ranking system of these variables with

different level of importance in such a way that a minimum number of quality variables needs to be observed. By finding the sufficiently high relationships between the unobserved and observed water quality variables, or between quality and quantity variables, the time series information can be transferred from the observed to the unobserved variables without additional sampling and analysis.

2.0 LITERATURE REVIEW

The analysis of water quality data has become one the important functions that the environmental engineer must perform. Expanding water quality programs and the advent of improved methodology for data acquisition have increased both the volume and the scope of the analysis to be carried out. Analysis is complicated by the fact that many of the underlying factors which influence variations in water quality are not well defined. These factors may be further obscured by the occurrence of random events. Consequently, the application of Time series analysis has become necessary. Several significant models were developed using the Time series analysis in many fields. However, only a few number of papers refer to the application of this approach in the field of water quality. The application of various approaches of Time series analysis in water quality modelling has been reviewed under the headings of approaches applied.

2.1 APPLICATION OF FREQUENCY ANALYSIS

Frequency based approach of time series analysis has been traditionally the one used in water resources engineering and it has been employed by several authors in water quality analysis. Probabilistic water quality analysis starts with classical, deterministic, water quality models of fate of pollutants and overlays probability theory in such a way that the probability distribution of the resulting receiving water concentration are computed. The following models are found to be based on frequency approach.

The problem of describing the profiles of organic

pollution and dissolved oxygen along a stretch, generally below a source of pollution such as a municipal sewage treatment plant was under the consideration of authors. The work of Streeter and Phelps (1925) on the Ohio River marked the beginning of the classical theory. Since then other works had included additional factors on the work of Streeter and Phelps. Dobbins (1964) combined the results of various published works.

All of those results gave, for any downstream point, one value for the pollution concentration and one value of the dissolved oxygen concentration. No work had been done till 1964, in which one considered the actual probability distribution of values. Having enough dissolved oxygen present on the average to assume a healthy fish population is not sufficient to prevent fish kills. In contrast to previous models a stochastic model was presented by Thayer and Krutchkoff (1967) which gave a probability distribution for both pollution and dissolved oxygen at any downstream point. In that work, as with the work of Dobbins and others, it was assumed that there were five major factors operating in the stream. The assumed rates were the same as assumed by Streeter & Phelps in their study on Ohio river (1925). Specially, these factors and rates were -

i) The pollution and dissolved oxygen decreased by the action of bacteria and the rate of deoxygenation was assumed to be proportional to the amount of pollution present i.e, the first order reaction takes place. Further, it was assumed that there was always some oxygen present in the system.

ii) The dissolved oxygen increased due to the process of reaeration at a rate proportional to the dissolved oxygen deficit.

iii) The pollution was decreased only by sedimentation and adsorption on the rocks with a rate proportional to the amount of pollution present.

iv) The pollution increased from small sources along the water course with a rate independent of the amount of pollution present.

v) The dissolved oxygen decreased at a constant rate due to the net effect of benthic demand, photosynthetic respiration, and the increase in oxygen due to the photosynthesis.

In addition to the five assumptions just mentioned above, one more was assumed that the changes in both pollution and dissolved oxygen occur in small units of size Δ . A quasilinear partial differential equation of the first order was developed by Thayer et al. (1967) to evaluate the joint probability of finding the system with the pollution in state 'm' and the dissolved oxygen in state 'n' at time 't' denoted by $Pr_{m,n}(t+h)$ as follows:

$$\begin{aligned} \frac{\partial P}{\partial t} = & - \frac{1}{\Delta} \left[L_a P + D_B P + K_2 C' N P + L_a S P + \frac{D_B}{R} P K_2 C' N R P \right] \\ & - \frac{\partial P}{\partial S} \left(K_1 S + K_2 S + K_3 + \frac{K_4}{R} \right) + \frac{\partial P}{\partial R} \left(K_2 R - K_2 R^2 \right) \\ & - \frac{1}{R} \left[\frac{D_B}{\Delta} + K_1 \frac{\partial}{\partial S} \right] P(S, O; t) \end{aligned} \quad (1)$$

in which $P = P(S, R; t)$. A probability generating function was defined as:

$$P(S, R; t) = \sum_{M=0}^{\infty} \sum_{N=0}^{\infty} Pr(t) S^M R^N \quad (2)$$

The solution of the partial differential equ.(1) was obtained for three different sets of initial conditions as given below.

(i) It was assumed that both the pollution and the dissolved oxygen states are known initially.(ii) For this case, it was assumed that there were a basic stream variability due to some pollution already in the stream and that the pollution concentration at $t=0$ is raised by a constant amount.

(iii) For this case, the initial variability was a complex combination of the effects of various sources of upstream pollution and the pollution entering at $t=0$. It was assumed that the pollution and dissolved oxygen states had independent binomial distributions where mean and variance can be measured.

With these three initial conditions the solution of the partial differential equation (1) had been obtained (Thayer et al 1967) by the authors, yielding the mean and variance for both of the amount of pollution and dissolved oxygen present.

It was noted that the equations for the mean amounts of pollution and dissolved oxygen as derived from the stochastic model of Thayer et al.,(1967) were identical to the equations of Dobbins (1964) which had been obtained from a deterministic differential equation approach. Furthermore, that model was applied to Sacramento River for the region below the city Sacramento for the prediction of dissolved oxygen and pollution at down stream points and found that the predicted results had a good agreement with the observed data.

Custer et al.,(1969) presented a temporal and spatial probability distributions of BOD and DO resulting from a single point source

of pollution. They had assumed all the five assumption as given in Thayer et al., (1967) stochastic model for BOD and DO in streams. As reported earlier the Thayer et al., work was based on Dobbin's model with the mechanisms effecting BOD and DO concentrations modified so as to be random in nature with one additional assumption in which the pollution and dissolved oxygen were discretized. The term was introduced to represent the optimum size and hence all transitions in BOD and DO were asserted to be in units of size. In this study this additional assumption was not taken in account. However, a single point source of pollution was taken under consideration, which according to author was not an added restriction, since the accumulative effect of several sources could be obtained by the principle of superposition according to which if two or more loads of pollution enter a volume of water the net effect is the sum of the individual effects. In order to apply this principle to oxygen it would be necessary to consider the oxygen deficit rather than the usually considered dissolved oxygen. However, the principle could be applied directly to BOD. In probabilistic terms the principle implied that the net distribution was the convolution of the individual distributions. The model was applied to an estuary considering all the random component which had been considered by Thayer et al., (1967). However, in this model diffusion had been considered as an additional random process. Further, the model considered all factors considered by Dobbins (1964) except: a uniform increase of BOD by land runoff; and a uniform decrease in dissolved oxygen due to the benthic demand. These two factors had been handled separately, and their combined effect was obtained by the principle of superposition. The model could be used to find

out the probability of the system being in any particular states of given pollution and dissolved oxygen by picking out the desired coefficients of $P(m,n,t)$ as evaluated by Thayer et al.,(1967).

Kothandaraman et al.,(1969) presented a probabilistic analysis of dissolved oxygen and biochemical oxygen demand relationship in streams for the following objective:

i) to examine the relative importance of the variations in the reaction rate coefficients affecting the bacterial oxidation of organic matter, and the atmospheric reareation, in predicting the dissolved oxygen responses of the receiving streams.

ii) to determine the nature of variations in reaction ratecoefficients and formulate and **test** hypotheses concerning their chances of variations.

iii) to develop a procedure for predicting the dissolved oxygen in a river at sites ,down stream of a waste source by taking into account the variations in the velocity coefficients.

iv) to enumerate quantitatively the chance of variations in dissolved oxygen responses in terms of probability measures.

In order to meet the first objective, a sensitivity analysis was made on the Streeter - Phelps equation for stream assimilative capacity. Sensitivity analysis applied to the concept in which all except due to the variables in a system were held constant and this single exception was allowed to vary through its full possible range and the effects on system performance were noted. If the measured output was found to vary significantly, the system was said to be sensitive to that variable for the given condition. The sensitivity of the system to the variation in K_1 and K_2 at different temperatures had also been made. Furthermore, the variation in K_1 and K_2 had been studied due to the probabilistic

variations in velocity of the stream. They investigated the nature of variation in K_1 values for the Ohio river samples and found that K_1 values vary according to the normal probability law. The probability distribution of K_1 was assumed to be Gaussian, defined as:

$$fk_1 = \frac{1}{\sqrt{2\pi}\sigma_1} \exp \left\{ -\frac{1}{2} \left(\frac{k_1 - \mu_1}{\sigma_1} \right)^2 \right\} \quad (3)$$

Since K_1 could not be negative, a truncated normal distribution was used to define the probability distribution of K_1 . A range of values for K_1 within the limits $(\mu_1 \pm 2\sigma_1)$ was found adequate for all practical purposes. Kothandaraman (1970) presented a study to enumerate quantitatively the chance variations in the ultimate first stage BOD after a stipulated interval of time, knowing the initial ultimate first stage BOD. The probability density function of ultimate first stage BOD at time 't' was obtained using equ.(3) (Kothandaraman et al., 1969) as given below:

i) for $L > 0$

$$fL = \frac{1}{\sqrt{2\pi} t \sigma_1} \frac{1}{L} \exp \left[-\frac{1}{2t^2 \sigma_1^2} \left\{ \ln(L) - \left(\ln(La) - t\mu_1 \right) \right\}^2 \right] \quad (4)$$

ii) for $L \leq 0$

$$fL = 0 \quad (5)$$

From Eq.(4) it is clear that the ultimate first stage BOD was log normally distributed under the assumptions that the bacterial oxidation of organic matter was a first order reaction, and that the deoxygenation coefficient had a normal distribution. The expression for evaluation of most probable values of ultimate first stage BOD(L) was given as:

$$MPV_L = \exp \left\{ \ln (La - t\mu_1) - \sigma_1^2 t^2 \right\} \quad (6)$$

Schofield and Krutchkoff (1972) developed a general stochastic model for BOD and oxygen deficit in segmented estuary. In this study, an estuary was defined as the tidal proportion of a river. As with any real world process, idealizing assumptions were made in order to proceed with any form of mathematical analysis. The following were the assumptions upon which this work was based:

- i) A one-dimensional process was assumed. The river or estuary was assumed consisting of uniform cross-sectional concentration and velocity profiles.
- ii) The fluid velocity in the estuary was approximated by the following law:

$$U(x,t) = U_F(x) + U_T(x) \sin(WTt), \quad (7)$$

in which:

$U(x,t)$ = velocity as a function of time and position;

$U_F(x)$ = fresh water velocity as a function of position;

$U_T(x)$ = maximum velocity as a function of position;

ω_T = tidal frequency ($\frac{2\pi}{12.5n}$) for estuaries, and 0 for rivers.

- iii) The Dobbins (1964) assumptions of first order reaction, deposition, and reareation rates were assumed.
- iv) Parameters, conditions, etc., were assumed to be constant with time. They were, however, made function of tidal phase appropriately, all parameters and conditions were made functions of position.

The probability generating functions for the probabilities of BOD and oxygen deficit concentrations were developed. The

probability of the system being in any particular state were obtained using eq.(7) .It was found that the developed model (Schofield et al.,1972) was much more general than the previous models and yielded excellent agreement with observed data when photosynthesis and other effects were not present.This model accurately represent estuary conditions, under very les limiting restrictions for a dynamic (non steady-state)eco system in a one-dimensional, eutrophic (pollution - enriched) estuary yielding a quantitative relationship between the causes (pollution discharge in to an estuary) and resulting effects (the wholesale degradation of the ecological environment). This cause-effect relationship included a random component which account for the stochastic nature of the process. For the application of this study the following limitations were imposed:-

- i) The analysis was restricted to a one dimensional system only. Therefore, the model could be used to describe rivers and estuaries which had velocity and concentration profiles comparatively uniform over their cross sections.
- ii) It was assumed that the behaviour of each pollution particle was independent of all other particles, i.e., the particles were stochastically independent. Therefore, the behaviour of a single particle and its corresponding probability density function (PDF) could be studied independently. The PDF for more than one conservative pollution particle could also be developed.

Padgett and Rao (1979) presented a technique for estimating the joint probability distribution of BOD and DO at any point along a stretch of stream based on n observed BOD and DO values under the same general assumptions as stated by Thayer and Krutchkoff (1967). In this study the use of nonparametric bivariate

probability density estimator had been described and the application of the density estimator to the pollution problem had also been presented. In particular, the techniques could be utilized to control the amount of waste input by the pollution source by specifying desired probability bounds on BOD and DO at a down stream point and finding the corresponding required bounds at the upstream end of the stretch.

Finney, Bowles, and Windham (1982) developed a one dimensional steady state probabilistic river water quality model to compute the river water quality in terms of joint and marginal probability density functions of BOD and DO at any point in a river. The model could simultaneously consider randomness in the initial conditions, inputs and coefficients of the water quality equations. Any empirical or known distribution could be used for the initial conditions. Randomness in each of the water quality equation inputs and coefficients was modelled as a Gaussian white noise process. The joint probability density function (Pdf) of BOD and DO was determined by numerically solving the Fokker-Plank random differential equation. In addition, moment equations were developed which allow the mean and variance of BOD and DO to be calculated independently of their joint pdf. The probabilistic river water quality model was examined through sensitivity study and an application to a hypothetical river system.

An analysis of the water quality response of a stream receiving intermittent storm runoff was carried out within a probabilistic framework by Dominic M. DiToro (1984). Log normally distributed runoff, streamflows, and concentrations were assumed and cross co-relations were obtained explicitly which were included in the exact solution method. An approximate moment

method was also suggested which was found suitable for rapid screening analysis.

Tung and Hathhorn (1988) presented an approximate ANDpractical methodology to assess the probability distribution of dissolved oxygen deficit based on the streeter-Phelps equation. The methodology involved the use of first order analysis of uncertainty of the DO deficit equation. The statical moments estimated were used in an appropriate probability distribution for the DO deficit concentration.

Tumeo and Orlob(1989) presented an analytical procedure using probability density function/moment (PDF/M) method as a tool for analysis of uncertaninties in models of environmental systems. It provided a capability for direct, efficient calculation of probability density functions for state variables and their moments. The method gave greater flexibility and lower computational effort than Monte Carlo simulation with equivalent or better estimates of moments of the distributions. Unlike methods for the solution of stochastic differential equations, the PDF/M method did not require that Gaussian distributions be assumed in the solution technique. Complex random functions of time and space could also be included.

A time series analysis approach was applied by Jayawandena and Lai (1989) to model 21 years of mean monthly water quality data in the Guangzhou reach of the Pearl river in southern China. The basic properties of the water quality data time series were determined. Time and frequency domain analysis were carried out, and the dependent stochastic component was represented by various stochastic models. Synthetic water quality data were generated using the probability distribution of the independent

residuals.

Statistical methods could be useful for the verification of mechanistic water quality simulation models. Thomann's paper (1982) is the best example of the application of statistical tests to assess model fit combined with practical guidance on the advantages and disadvantages of reliance on the statistical measures of fit. Reckhow, Clements, and Dodd (1990) extended Thoman's analysis and recommendations with guidance on the appropriate structure and application of statistical tests to assess model fit. In addition, consequences and corrective measures associated with assumption violations have been examined. The t-test, the Wilcoxon test, regression analysis, and the Kolmogorov-Smirnow test have been extensively described and applications of each were presented for the verification of a mechanistic water quality model.

2.2 FOURIER AND SPECTRAL ANALYSES

Spectral analysis, sometimes called 'spectrum analysis', is the name given to methods of estimating the spectral density function, or spectrum, of a given time series. Spectral analysis is essentially a modification of Fourier analysis so as to make it suitable for stochastic rather than deterministic functions of time. Fourier analysis is basically concerned with approximating a function by a sum of sine and cosine terms, called the Fourier series representation. Following models have been developed employing the Fourier analysis.

Thomann (1967) presented some of the techniques of analyses of time series records using the general theory of Fourier and spectral analyses with special reference to the temperature and dissolved oxygen variability for the Delaware

Estuary. Other variables such as sunlight intensity and sewage treatment plant effluent had also been examined. This was followed by an evaluation of Fourier and power spectrum computations and how these techniques could be used as tools towards a further understanding of the physical environment. The results of applying these analyses to temperature and dissolved oxygen time series were given in table 1. and power spectrums of dissolved oxygen and temperature in following figures(fig.6, fig.7, and fig.8).

Wastler et al.,(1968) presented a spectral approach to study the estuarine behaviour especially to predict the effects of reduced inflow from the major tributary stream on the quality of water in the Harbor. The problem involved; first the establishment of the existing quality patterns; second the prediction of the estuary's hydraulic behaviour under proposed conditions of reduced inflow, and thirdly the determination of the future changes in both the contaminant distribution and water quality. For this, a time series analysis of sequential records of river inflow and chloride concentration was selected as the most promising approach for characterizing the behaviour of the estuary. The sampling program developed for providing the necessary data involved the collection of samples from selected sites on a frequency less than the period of the predominant environmental forces, the tide. A series of six intensive surveys was conducted to provide 30 point records with a 4 hour frequency at different flow rates. These records were subjected to an analysis of variance to ensure that they represented separate populations. The independence of each record was established and cross spectral analysis were carried out on every pair of chloride

concentration and stream flow records. The technique of cross spectral analysis was conceptually a harmonic covariant analysis of two time-series records, where one record was considered a causative factor and the other a resultant. In this case, the fresh water inflow was considered the cause and the chloride concentration was considered as the effect. The statistics produced highlighted the significance of the cause-effect relationships as well as the temporal relationship. The computational steps for cross-spectral analysis were: i) computation of the individual power spectrum of each records; ii) computation of the cospectrum and quadrature spectrum from the cross correlations of the two records;

iii) computation of the coherence, the phase lag and the response spectrum from the four spectra computed in steps (i) and (ii); and iv) computation of the overall response.

Each of these steps had been discussed in detail (Wastler et al., 1968).

Robert V. Thomann (1970) applied a Time Series analysis to several existing municipal waste treatment plants data for the following objectives:

(i) to gain further insight into the nature of the variability of flow and biochemical oxygen demand (BOD),

(ii) to develop additional measures of performances of treatment plants which might be proved useful in estimating future variability; and

(iii) to relate the behaviour of the treatment plants to the resulting stream quality variations.

The author applied the Fourier and spectral analysis and determined quantitatively the amplitudes and phase angles of the

important periodic components and the contribution to the total variance of each of the harmonics and concluded that the maximum dissolved oxygen variability would occur at the location of the critical dissolved oxygen deficit.

Kothandaraman (1971) presented a study for the analysis of water temperature variations in large rivers with the primary aim to prepare a report for an investigation regarding the nature of seasonal and non-seasonal variations in the daily mean river water temperature at a given location and to develop a method for the prediction of water temperatures based on observed meteorological data. Such a predictive model for naturally occurring water temperature variations was found invaluable for predicting the responses of water bodies to any addition or alterations imposed by power plant operations. For this particular study a 4-yr record of the daily mean water temperatures of the Illionois river were collected at Peoria, Illinois. Kothandaraman et al.,(1970), Thomann (1967), and Ward (1963) had studied the annual temperature vaviations in rivers and impoundments and conmlcluded that a harmonic with a periodicity of 1 year was suitable for fitting the water temperature data in lakes, estuaries, and rivers accounting for about 95% of the total variance. In order to seperate the cyclic or seasonal variations from the observed data, fourier analysis was carried out. After removing the seasonal variations from the observed data, the nature of non seasonal or random variations were investigated by applying the Fourier Analysis.

2.3 APPLICATION OF BOX-JENKINS METHOD

An innovative approach to time series analysis had been

developed by Box and Jenkins (1970). It has time as its basis as opposed to frequency, the basis for frequency analysis. The time based approach to time series analysis attempts to fit a model by expressing the time series as the output from a linear filter having a random input and consisting of several transfer functions in series. Further, the method uses a minimum number of parameters. The following studies have been done using the Box-Jenkins method.

Wallace and Zollman (1971) presented an interesting investigation of time varying organic loads in a municipal treatment system. The authors demonstrated the application of some methods of mathematical modelling introduced by Box and Jenkins (1972) for time series analysis of data. The primary tools for data analysis are the plots of the original time series and the logged autocorrelation coefficients of the original data and their difference. Simple methods had been identified and best estimates of parameters as well as diagnostic checks of the model were made. The authors concluded that the procedure was found to depend heavily on the interpretation of a graphical picture of data and its auto correlation function as well as on the auto correlation function of the model residuals. Although there was sometimes an attempt to avoid the data plotting and to merely examine the tabulated numbers, this practice often leads to errors or delays in understanding.

Huck and Farquhar (1974) undertaken a study to examine the applicability of the Box-Jenkins method to the modelling of water quality data. Early applications of the Box-Jenkins method to the water resources area were undertaken by Carlson and Co-workers (1970). They developed parametric models for annual streamflow data

and achieved significant reductions in variance with one or two parameters. In addition, they employed the model for forecasting also. McMichael and Hunter (1972) developed models temperature and flow in rivers. Their model incorporated both deterministic and stochastic components, the later being obtained by the Box-Jenkins method. They found that this type of model to be preferable from a numerical and a rational point of view to a purely stochastic or purely deterministic model. McMichael and Vigani (20) applied Box-Jenkins approach to the municipal treatment system organic loadings as discussed earlier. In the present study the following conclusions were drawn by the authors

- i) The Box-Jenkins method for time series analysis was successful in modelling the hourly water quality data recorded in the St. Clair River near Corunna. The models were parsimonious and physically reasonable. They explained 60% - 70% of the observed variation and produced good forecast.
- ii) The Box-Jenkins method did not require that the data be stationary, which was an essential condition for application of frequency approach .
- iii) The Box-Jenkins methods was able to employ on defective data also, containing an oscillation.
- iv) The Box-Jenkins method provided the water quality analyst with a new technique which may succeed where other methods would not. It can also serve as an alternative, and perhaps superior, approach in situations where other methods can be employed.

Box-Jenkins time series analysis for the monthly water quality data in Chung-Kang River was conducted by Lohani and Wang (1987) and developed several significant models. Early applications of the Box-Jenkins method to the water resources area

were undertaken by other researchers but they considered one or two parameters only. Carlson et al (1970) developed parametric models for annual streamflow data with one or two parameters. McMichael and Hunter (1972) developed models for daily temperature and flow in rivers. Huck and Farquhar (1974) used Box-Jenkins techniques in modelling the hourly data of Chloride and dissolved oxygen. Lohani and Wang (1987) described the application of Box-Jenkins modelling for twelve monthly water quality parameters e.g. temperature, turbidity, specific conductance, total alkalinity, pH value, total solids, suspended solids, chloride, sulphate, ammonia nitrogen, dissolved oxygen, and biochemical oxygen demand. They analyzed monthly samples taken at three stations for all the parameters mentioned above. Five years of data (1976-1980) were used for the comparison of the results forecasted using the time series models developed using the Box-Jenkins time series analysis.

2.4 APPLICATION OF MULTIVARIATE TECHNIQUES

The data from river basins usually involve a number of variables and hence the interpretation through standard statistical techniques is not satisfactory and usually requires a multivariate approach. For example, an n variable vector would lead to n means, n standard deviations, and $(n^2 - n)/2$ correlation coefficients; or a total of $(3n + n^2)/2$ statistical parameters subject to interpretation. If n were equal to 20, this would mean 230 parameters would have to be analyzed. The advantage of using multivariate techniques lies in the fact that the number of statistical parameters subject to interpretation is reduced significantly with the concomitant reduction of large data bases

to a manageable level for the purpose of analysis. Two problems which arise in the use of any statistical analysis are missing data values and satisfaction of the various assumptions concerning the data which allow the use of a specific statistical technique. Various techniques presently exist for handling missing data values but all of them can not be applied successfully to the water quality data values.

Mahloch (1974) demonstrated the application of multivariate statistical techniques to the analysis of water quality data and presented a method for handling missing observations. The results of the study indicated that a simultaneous, multiple regression technique could be used for supplying missing data and that at any particular level the entire data matrix could be considered, thus reducing the computational efforts. The applications of the multivariate techniques examined in this study centre on either extracting information from the data or testing hypotheses which would arise concerning the data. Principal components and factor rotation could be used to reduce the original set of data variables to a group of factors which explain water quality states and the major levels of effects on water quality. Canonical correlation could be used to ascertain if a relationship existed between a set of conceptually different water quality variables such as biological indicators, physical, and chemical parameters. The canonical analysis could also be used to show which parameters in the data sets contribute most heavily to the interrelationship. Partial correlation could be used to test whether a reduced set of variables would be used to explain the variation in the water quality data matrix. Additionally, it could be used to remove the effect of control set of variables from the

remaining water quality parameters. The MANOVA and discriminant analysis are techniques which test differences in water quality observations at the population level. These techniques could also aid in elucidating the parameters most responsible for differences between the observations. Therefore it can be concluded that the use of multivariate statistical techniques is a very important tool for meaningful water quality data analysis. Since the quality and quantity of reliable water quality data are increasing, an investigator should avail himself of these techniques to facilitate any interpretation of these data. To ignore these techniques would be denying the analyst a powerful tool in the interpretation of water quality status for a region.

2.5 APPLICATION OF UNCERTAINTY ANALYSIS

Water quality models are mathematical construction which integrate a number of complex phenomena as water transport, reaction kinetics, and external loadings. There is always some error or uncertainty in a model. A mathematical model can not represent the real process perfectly; either there is some unknown process involved or some part of the representation can not be calculated due to the complexity or economics. The uncertainty has usually been attributed to the randomness inherent in natural processes. The following studies have been done taking the effects of parameter uncertainty in stream water quality modelling in to consideration.

Peter and Parker (1983) presented an approach to estimate the uncertainty of the output of a model. Three types of errors in modelling were defined by Young and Turney (1976). Model error or conceptual error introduced by the failure of the mathematical model to describe accurately what occurs in nature;

sampling and measurement errors associated with the sampling and measurement techniques for data input to the model; and the phenomenological error introduced by the stochastic nature of environmental processes. The purpose of this study was to examine, for a parameter that had a log normal probability distribution and could be expressed by an exponential or first order decay and the relationship between the uncertainty of an estimate at a certain time or location and the number of samples on which that estimate was obtained. A methodology had been presented to calculate the probability that the true value of a parameter that was being estimated exceed some upper limit, even though the value of this parameter estimated from measurements could be below this limit. This probability was of primary importance in deciding if the results from the last cycle were satisfactory or if more samples should be collected and analyzed.

The effect of input parameter uncertainty on model output uncertainty was investigated by Warwick and Cale (1986). The mathematical model selected for investigation assumed a one dimensional, steady state, and uniform flow conditions including longitudinal dispersion. Hydraulic input parameters (flow rate, velocity, and longitudinal dispersion) were assumed to be constant with respect to both time and space. Uncertainty in these hydraulic parameters, which results from in-stream measurements error, was characterized with normal distributions. First order reaction rate uncertainty was assigned a bounded uniform distribution to signify a general knowledge of an expected range for highly reactive and relatively inert organic priority pollutants.

2.6 APPLICATION OF RANDOM DIFFERENTIAL EQUATIONS

The theory of random differential equations has been used successfully in river water quality modelling assuming stochasticity in the form of an additive random disturbance $s(t)$. In the following studies the random differential equation have been used in the modelling of stream water quality.

Padgett (1977) used the Streeter-Phelps equations with initial values of BOD and DO represented by random variables defined by Gaussian distribution. Non-point source loadings were modeled as uniform deviates and all other rate parameters were assumed constant. Tiwari (1978) used 16 first order differential equations and rate constants to model an aquatic eco-system. The initial conditions and rate constants were all defined as random variables with Gaussian distributions. Padgett and Finney et al. (1982) solved the Streeter Phelps equations by interpreting the Fokker-Plank equation to determine the joint probability distribution function of BOD-DO. Finney et al. tried several different combinations of standard deviation parameters while Padgett used a standard Gaussian distribution and bivariate distributions with different correlation coefficients.

A stochastic model for dissolved oxygen in a river was developed by Dewey (1984) to examine the effect of various management options on the DO levels in river. The method for determining the dissolved oxygen (DO) level in a river was based on modifications of a set of random differential equations to include nitrogenous oxygen demand (NOD) and the DO responses after Streeter and Phelps. The method assumed randomly generated rate constants and input parameters which were described by probability distributions determined from Survey data means and

their standard deviations to generate the probable dissolved oxygen levels in a river. The model was applied to the Thames river, London, Ontario, to determine if flow augmentation would replace the number of episodes of low dissolved oxygen in the river during the low flow seasons. In addition, the model was used to test if improved treatment in the water pollution control plants would alleviate the low dissolved oxygen level in the river. The model was also used to test the solution's sensitivity to the rate constants. The method of testing for sensitivity was performed as follows. Firstly, a simulation was made with all random variables kept to within row distribution by specifying a very small standard deviation on each random variable. Then, for each random variable, one per run, the distribution of that particular variable was given a large deviation based on 25 percent of the mean value. Now, choose a particular location in each reach and plot the maximum and minimum level for both the very small deviation and the large deviation variable.

Leduc, Unny and Mc Bean (1986) presented a stochastic model of first order BOD kinetics. Based on the mathematical theory of stochastic differential equations and assuming first order kinetics, analytical expressions were derived for models of the temporal mean and variance in the BOD curve. Complex environmental phenomena inherent to BOD progression provided a sound basis to introduce a stochastic term into the deterministic, first-order BOD formulation. The stochastic term was then approximated by a Gaussian white noise term. The analytical formulae had been derived using the stochastic techniques to moment equation, the Fokker-Planck equation, stochastic integration, and the Riccati equation.

A one dimensional steady state stochastic waterquality model was developed by Zeilinski (1988) for the computation of the mean values and standard deviations of CBOD, DO and NBOD concentrations at any point in a river. The model considered randomness in the initial conditions, inputs, rate constants, and other model parameters as well as randomness in each of the modelled processes themselves. The stochastic characteristics were determined by analytically solving the moment equations associated with stochastic differential equations. The solution was obtained for a diurnally varied photosynthetic component. The resulted equations could be readily solved on micro-computers and consequently could be used effectively in an interactive model for river basin planning.

2.7 APPLICATION OF STOCHASTIC MODELS TO WATER QUALITY MANAGEMENT

Several researchers have solved water quality management problems in the deterministic context (i.e., all parameters considered are constant or known with certainty). However, to come closer to real life situations a chance constrained modelling should be formulated considering both the stream flow and stream quality as a random variable. Following stochastic water quality models have been developed in the field of water quality management by various workers.

A methodology for reflecting stochastic considerations in an optimization was presented by Burn and McBean (1985). The technique using chance constrained programming, was applied to a water quality management problem considering the inter-reaction between biochemical oxygen demand (BOD) and the dissolved oxygen (DO) concentration in a river. The uncertainty in the problem was considered to be embodied in transfer coefficients for which a

lognormal distribution was derived from moment estimates provided by first order uncertainty analysis.

A stochastic optimization, simulation method was presented by Ellis, McBean and Farquhar (1985) for delineating least cost treatment sequences for a centralized liquid industrial waste treatment facility. A dynamic programming model was used to perform the optimization. The function of the model was to delineate least cost treatment sequences that would produce an acceptable effluent stream quality given a probabilistically-generated influent waste regime. The model was structured to permit the following user-determined options, waste types and respective volumes in the waste inventory, specific contaminants with in each waste types, contaminant specific probability density functions for waste strength; unit treatment processes including performance efficiencies and related costs; and individual contaminant effluent standards. The stochastic dynamic programming model was used as a screening device, identifying unit treatment processes and sequence of processes with favourable cost-effectiveness attributes.

Fujiwara, Ghanendran, and Ohgaki (1986) presented a chance constrained model dealing the river quality management under stochastic streamflow. This model was concerned with the problem of optimally allocating treatment efficiencies among several waste water discharges along a river, such that a prespecified dissolved oxygen stream standard would be maintained at a minimum cost to the region as a whole. The stream flow was recognized as a random variable with a known probability distribution. This model overcome a major drawback of Lohani and Thanh's model (1978), namely the requirement of a prior knowledge of the initial DO

deficit at the top of every reach. This was not, however, logical to assume values for these DO deficits because they were a consequence of the treatment policy in the upstream reaches, which was yet to be specified, thus the assumed dissolved oxygen deficit could not be used as data to determine the optimal policy in the first place.

A chance constrained stochastic programming model was developed by Ellis (1987) for water quality optimisation determining the list cost allocation of waste treatment plant biochemical oxygen demand removal efficiencies, subjected to probabilistic restrictions on maximum available in stream dissolved oxygen deficit. The model extended well beyond the traditional approaches that assumed stream flow as the sole random variable. In addition to stream flow, other random variables in the model were initial instream BOD level and dissolved oxygen deficit; waste outfall flow rate; BOD levels and BOD levels and DO deficits; deoxygenation, reaeration, and sedimentation scour rate coefficients of the Streeter Phelps DO sag model; photosynthetic input-benthic depletion rates and nonpoint source BOD input rate for the Dobbins extensions to the Streeter Phelps model. These random variables appeared in more highly aggregated terms which in turn form part of the probabilistic constraints of the water quality optimization model. Stochastic simulation procedures for estimating the probability density functions and covariances of these aggregated terms were formulated. A chance constrained programming variant, imbedded chance constraints, was presented along with an example application. In effect, this method imbedded a chance constraint within a chance constraint in a manner which was loosely associated with the distribution free method of chance

constrained programming. It also allowed the selection of nonexpected value realizations of the mean and variance estimates employed in the deterministic equivalents of traditional chance constrained models. As well, it could be used as a convenient mechanism for generating constraint probability response surfaces. A joint chance constrained formulation was also presented illustrating the possibility for prescription of an overall system reliability level, rather than reach by reach reliability assignment.

Canale and Effler (1989) developed a probabilistic phosphorus model that utilizing the Monte Carlo technique and applied to address water quality management issues for Onondaga Lake. Simulations with the probabilistic model had been used to evaluate the significance of year to year changes in rainfall, the level and variability of point sources and uncertainty in the model coefficients.

Fujiwara, Puangmaha, and Hariaki (1989) presented a study related to river basin water quality management in stochastic environment. They modified the stochastic water quality management model of Burn and McBean (1985) which considered various river parameters as a random variables and optimizing wastewater treatment efficiencies at source points. A monte carlo simulation was used to calculate quantities of random variables concerning DO concentration instead of the first order uncertainty analysis. With an objective of maintaining violation of water quality standards with in maximum allowable probability levels, an iterative procedure for optimization and simulation was proposed. A simulation analysis was used to calculate the probability of violating the DO deficit standard at each checking point.

The effect of correlation among the input parameters and variables on the output uncertainty of the Streeter-Phelps water quality model was examined by Song and Brown (1990). Three uncertainty analysis techniques were used: sensitivity analysis, first order error analysis, and Monte Carlo simulation. A modified version of the Streeter-Phelps model that includes nitrification, net algal oxygen production, and sediment oxygen demand was used. Analysis were performed for a wide variety of simulated stream flow conditions.

3.0 CONCLUDING REMARKS

In planning a water pollution control program in rivers, the analysis of the existing water quality parameters and the prediction of the changes in future is an important step. To make wise choices in expanding the nation resources for the prevention and control of water pollution, it is necessary to first understand the relationship between the discharge of pollutants in a body of water. Once the cause effect relationship is known the effectiveness of a prospective pollution control investment can be evaluated before the investment is made. In this way the best of many alternate control scheme could be selected for a given locality, based on the needs, resources and conditions of the locality. Usually this cause effect relationship is expressed in the form of a mathematical model where each known step, process, mechanism, etc. is represented by a corresponding mathematical analog.

The water quality variations in a river may be modelled by the deterministic approach, in which the cause-effect relationships are represented by differential equations or by the stochastic approach, in which the variation of the magnitude of one or more parameters of water quality is represented as a function of time or space.

The deterministic approach is found suitable for predicting the steady state water quality condition along a river and to predict the short term transient state of a water quality parameter, whereas, the stochastic approach enables the identification of trends and periodic phenomena present in natural

data series, their decomposition, and subsequent synthesis for data generation and forecasting.

A major portion of the complexity associated with water quality modelling and prediction is the inherent randomness exhibited throughout the stream environment. Not only, the physical and biological processes are clearly defined, but also an imposing number of uncertainties are associated with the various process occurring within the system environment. Due to the general variability, uncertainty, and unpredictability of pollution and purification processes in streams there is a great need for developing the water quality models using the stochastic or probabilistic approaches.

Based on the literature reviewed, the following comments are made:

i) The most of the application of stochastic modelling in the field of water quality has been made in foreign countries. Hence, there is an urgent need for taking up the studies related to modelling of water quality parameters using stochastic approach for Indian rivers.

ii) In context of developing countries like India where there is a large scope of future developments, it is highly obvious that the data will be passing the nonstationarity which should be removed using an appropriate methodology before proceeding for the further analysis.

iii) The application of stochastic approach in modelling of river water quality, needs the availability of sufficient reliable water quality data taken after a regular interval (hourly, daily, or monthly etc.) depending up on the purpose of study. Hence a continuous monitoring of water quality parameter is

highly essential. Now a days, a number of modern techniques and the development of automation using electronics are available which permit the application of more precise method for contineous water quality monitoring.

iv) Low flow determination is very important for designing the waste treatment facilities. The waste loadings that may be imposed up on a stream without deleterious effects, is closely related to the low flow regime of the stream. The stochastic approach can be used for modelling the water quality parameters in low flow situations and in predicting the probable range of water quality parameters and their consequences during the expected pollution loading and low flow conditions.

v) For the application of stochastic approach in the modelling of various parameters of water quality, it is highly essential to have a suitable and adequate data storage and retrieval system. The system should have a uniform and feasible storage format. The system should also be capable of storing the data in logical locations in form of statistical parameters representative to original data for easy retrieval and minimum memory requirement.

vi) The stochastic water quality models can be used to forecast the future probable values of various water quality parameters which can be utilized in evolving the stream/effluent standards based on various beneficial uses of river water for its different reaches having different flow and pollution loadings. Furthermore, the future forecasts can also be used to make the alternate arrangements as a safely measure in situations when the standards are violated.

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APPENDIX.-II Notations

- DO = Dissolved oxygen;
- BOD = Biochemical oxygen demand;
- $Pr_{m,n}(t+h)$ = Probability of system with the pollution, in state 'm' and dissolved oxygen in state 'n' at time 't';
- K1 = Deoxygenation rate coefficient;
- K2 = Reareation rate coefficient;
- K3 = Rate of decrease of pollution by sedimentation and adsorption;
- La = Ultimate first stage BOD;
- C_N = Dissolved oxygen in state N;
- C_N' = Maximum possible amount of dissolved oxygen in state N;
- DB = discretized unit of D.O.;
- t = time;
- f_{k1} = Probability distribution function for K1;
- f₂ = Probability density function for ultimate first stage BOD;
- MPV = Most probable value;
- U(x,t) = Velocity as a function of time & space;
- UF(x) = Fresh water velocity as a function if position;
- UT(x) = Maximum velocity as a function of time;
- ωt = Tidal frequency;

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