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ANALYSIS AND INTERPRETATION OF STOCHASTIC WATER QUALITY DATA USING PARAMETER ESTIMATION AND SPECTRAL ANALYSIS TECHNIQUES

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CHAPTER 1

INTRODUCTION

The increasing public awareness of environmental quality has created a need for continuous monitoring of our rivers and streams to identify compliance with water quality standards and to assess the existing water quality conditions. It has been reported (Sayers, 1971) that at least 10,000 monitoring stations are required on both interstate and intrastate waters to provide adequate coverage of the nation's water resources. Collection of data on the water quality variables is only part of the task. The wealth of data obtained from these monitoring stations need to be analyzed and interpreted in a meaningful and timely fashion for appropriate follow-up action.

The present state of the art of data collection and analysis leaves much to be desired. The philosophy of analyzing such data from a deterministic view-point has recently come under severe criticism (Thayer and Krutchkoff, 1966). This is understandable because stream water quality data are stochastic in nature. Such data are constantly affected by natural uncertainties caused by local weather and hydrological conditions and artificial events, such as recording errors, superimposed on them.

This investigation seeks approaches to analyze and interpret stochastic water quality data and study critically the applicability of the results to water quality monitoring.

An important aspect of this investigation is the analysis of the nature of the random events affecting water quality and their influence on the various water quality data and parameters. The effect of the random events on the water quality parameters may be studied through computer simulation. Available mathematical models may be used in simulation studies to represent the deterministic signal of the stream. The random events can be simulated by superimposing computer generated random noise on the deterministic signals of the stream. The resulting data can be used to estimate the parameters appearing in the model equations used in the simulation.

The number of monitoring stations is an important factor in collecting data for parameter identification in water quality models. It is highly desirable to develop procedures for parameter estimation such that the number of monitoring stations employed is minimum. In this way the selected procedure will be useful in designing monitoring schemes which play an important role in the economics of water pollution control programs.

Chapter 2 of this dissertation provides a critical review of the available literature in water quality modeling. It includes the development of the models, parameter identification and application of spectral analysis techniques in the analysis of water quality data.

In Chapter 3, it is shown that parameters may be theoretically estimated by employing time series data collected at only two monitoring stations and using a minimum number of data points. In Chapter 4, methods for estimating parameters are evaluated, based on results obtained in Chapter 3. Chapter 4 includes analysis of a model system with stochastic input and a model system with noise corrupted output measurements.

The influence of random events on water quality data may also be studied by applying spectral analysis techniques to field data. However, severe chance events such as instrument breakdown, violation of waste discharges, etc., make it difficult to correctly interpret the results from spectral analysis of field data. Therefore, it is desirable to conduct experiments under controlled conditions to gain additional experience in analyzing and interpreting such complex data. An experimental simulation of stream response to monitored inputs and the result of such a simulation are described in Chapter 5. Spectral analysis techniques were employed. The applicability of some of these results to water quality monitoring is discussed in this chapter.

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CHAPTER 2

REVIEW OF LITERATURE

2.1 INTRODUCTION

An important consideration in water pollution control is the development of mathematical models to aid in the analysis of water quality. This can either be achieved based on a knowledge of mechanism affecting the purity of natural bodies of water or be carried out by means of time-series analysis. These models describe the variations of water quality in terms of physical and chemical parameters. Such parameters must be known when the models are employed for prediction purposes.

A brief review on water qulaity modeling is presented in this chapter, It includes the development of the models, parameter identification, and applications of spectral analysis techniques in the analysis of water quality data.

2.2 WATER QUALITY MODELS

The development and use of comprehensive models for the management of water quality in river basins has been a subject of considerable interest (see Table 2.1). In earlier work, Streeter and Phelps (1925), considered the spatial distribution of BOD (which gives a measure of the amount of pollution) and DO concentrations governed by two mechanisms. They are: (a) the pollution decrease by the action of bacteria, and subsequent decrease in oxygen concentration and (b) the oxygen increase by reaeration from the atmosphere. In their model, the following assumptions were made:

(1) The stream flow is considered to be steady and uniform.

(2) The process along the entire stream is considered to be a steady state process, that is, for any given distance downstream the stream cross-sectional behavior at that point remains unchanged with change in time. This assumption

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Table 2.1 Summary of Deterministic Mathematical Models Used in Water Quality Management

Investigators	BOD	DO
Streeter and Phelps (1925)	$\frac{dL}{d\tau} = -k_1 L \, , \quad \tau = \frac{x}{U}$	$\frac{dC}{d\tau} = -k_1 L + k_2 \, (C_s - C)$
Camp (1963)	$\frac{dL}{d\tau} = -k_1 L - k_3 L + L_a$	$\frac{dC}{d\tau} = -k_1 L + k_2 (C_s - C) + P$
Dobbins (1964)	$D_L \frac{d^2 L}{dx^2} - U \frac{dL}{dx} - k_1 L - k_3 L + L_a = 0$	$D_L \frac{d^2 C}{dx^2} - U \frac{dC}{dx} - k_1 L + k_2 \, (C_s - C) - D_B = 0$
O'Connor (1967)	$L'_x = L_0 \, e^{-j_r \phi(x)} \, , \; U_0 = \frac{q}{A_0}, \; \phi(x) = \frac{x^2 - x_o^2}{2x_o}$ $N_x = N_0 \, e^{-j_n \phi(x)} \, , \; j_r = \frac{k'_1}{U_0}, \; j_n = \frac{k''_1}{U_0}$	$\frac{\partial C}{\partial t} = - \frac{q}{A_x} \frac{\partial C}{\partial x} + k_2 \, (C_s - C) + P(x,t) - k'_1 L'_x$ $- k''_1 N_x - R(x,t) - D_B(x,t)$
Thomann (1967)	$\frac{\partial L}{\partial t} = - \frac{1}{A} \frac{\partial}{\partial x} (qL) + \frac{1}{A} \frac{\partial}{\partial x} (D_L A \frac{\partial L}{\partial x}) \pm \Sigma_L$	$\frac{\partial C}{\partial t} = - \frac{1}{A} \frac{\partial}{\partial x} (qC) + \frac{1}{A} \frac{\partial}{\partial x} \, (D_L A \frac{\partial C}{\partial x}) \pm \Sigma_C$

Table 2.1 Continued

Investigators	BOD	DO
Dresnak and Dobbins (1968)	$\frac{\partial L}{\partial t} = D_L \frac{\partial^2 L}{\partial x^2} - U \frac{\partial L}{\partial x} - (k_1 + k_3) L + L_a$	$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - k_1 L + k_2 (C_s - C) - D_B$
Fan et al. (1971)	$D_L \frac{d^2 L^i}{dx^2} - U^i \frac{dL^i}{dx} - k_1^i L^i - k_3^i L^i + L_a{}^i = 0$	$D_L \frac{d^2 C^i}{dx^2} - U^i \frac{dC^i}{dx} - k_1^i L^i + k_2^i (C_s^i - C^i) - D_B^i = 0$
Shastry et al. (1973)	$\frac{dL}{d\tau} = - \frac{k_1 LC}{K_L + L} - k_3 L + L_a$	$\frac{dC}{d\tau} = - \frac{k_1 LC}{K_L + L} + k_2 (C_s - C) - D_B + P_m \{ \frac{1}{\pi} + \frac{1}{2} \sin 2\pi(\tau - t_s) - \frac{2}{3\pi} \cos 4\pi(\tau - t_s) \}$

merely implies that the stream geometry and characteristics at a given location are not altered significantly with time.

(3) The BOD and DO quantities are uniformly distributed over each cross-section, thus allowing the BOD and DO equations to be described by a one-dimensional flow model.

The limitations of this model led other investigators to modify the model in order to account for other factors affecting stream quality. Camp (1963), incorporated the decrease of BOD concentration by sedimentation, the addition of BOD concentration by local runoff and the increase in DO concentration by photosynthetic action (See Table 2.1) into the Streeter-Phelps model. Later, Dobbins (1964) improved Camp's model by adding the effect of longitudinal dispersion. O'Connor (1967), considered the spatial distribution of BOD as the contribution of carbonaceous BOD and nitrogenous distributions, and included the algal effect on the spatial and temporal distribution of the DO concentration. Thomann (1967), presented a more general form of the equation that describes the temporal and spatial distribution of BOD and DO concentrations. He considered the dispersion coefficient together with the stream cross-sectional area as functions of distance and time. At this stage, the initial assumptions made in developing steady state models have been modified drastically in order to represent changes in stream characteristics as close to the actual changes as possible. A year later, Dresnack and Dobbins (1968) presented a model which describes the temporal and spatial distribution of BOD and DO concentrations based essentially on the model given by Dobbins (1964).

Fan et al. (1971) extended Dobbins' (1964) model to predict BOD and DO profiles in a stream having several outfalls of waste and intakes of water. Changes in stream parameters were considered by dividing the stream into several segments and changing the parameters of the BOD and DO equations as needed in each segment. Shastry et al. (1973) presented a model which included nonlinear terms in the BOD and DO equations.

In recent years there has been a great deal of concern about the thermal pollution of rivers, lakes and seas by industrial activity. Davidson and Bradshaw (1967) (see Table 2.2) used a steady state model of BOD and DO together with the steady state model of the thermal energy to demonstrate the manifestation of a theoretical, optimal temperature profile which renders the DO a maximum at every point downstream from a single source of pollution. They used the nonlinear function given by Delay and Sanders (1966) and Edinger and Geyer (1965) to represent the net energy transfer rate Q. Dysart, III, and Hines (1970) presented an approach to water quality control for the case where there could be significant interaction of thermal wastes with organic wastes in a stream. A free-flowing stream which receives thermal and organic wastes was modeled as an N-stage serial system. The model used in their work (see Table 2.2) was similar to the model used by Davidson and Bradshaw (1967) except that the function used to represent the net energy transfer rate was linear.

Fan et al. (1971) presented a model which included the transient energy equation as well as the temporal and spatial distribution of BOD and DO concentrations (see Table 2.2). This model was used to determine an optimal cooling water discharge policy of a power plant. Fan and Hong (1972) used the steady state one dimensional dispersion model of BOD and DO given by Dresnack and Dobbins (1968) to develop a methodology for the preliminary design of a cooling water outfall system (see Table 2.2).

Table 2.2 Non-Isothermal Models Used in Water Quality Management

Investigators	Model Equations*
Davidson and Bradshaw (1968)	$\frac{dT}{d\tau} = \frac{rU}{\rho C_p q} Q$
	$\frac{dL}{d\tau} = - k_1 L$
	$\frac{dC}{d\tau} = - k_1 L + k_2 (C_s - C) + \langle P-R \rangle$
Dysart, III, and Hines (1970)	$\frac{d(T - T_e)}{d\tau} = - K (T - T_e)$
	$\frac{dL}{d\tau} = - k_1 L$
	$\frac{d(C_s - C)}{d\tau} = k_1 L - k_2 (C_s - C)$
Fan et al. (1971)	$\frac{\partial T}{\partial t} = D_L \frac{\partial^2 T}{\partial x^2} - U \frac{\partial T}{\partial x} + \frac{rU}{\rho C_p q} Q$
	$\frac{\partial L}{\partial t} = D_L \frac{\partial^2 L}{\partial x^2} - U \frac{\partial L}{\partial x} - k_1 L$
	$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - U \frac{\partial C}{\partial x} - k_1 L + k_2 (C_s - C) - \langle P-R \rangle$
Fan and Hong (1972)	$D_L \frac{d^2 T}{dx^2} - U \frac{dT}{dx} + \frac{rU}{\rho C_p q} Q = 0$
	$D_L \frac{d^2 L}{dx^2} - U \frac{dL}{dx} - (k_1 + k_3) L + La = 0$
	$D_L \frac{d^2 C}{dx^2} - U \frac{dC}{dx} - k_1 L + k_2 (C_s - C) - D_B = 0$

*The parameters k_1, k_2, C_s, and $\langle P - R \rangle$ are functions of temperature.

In general, the deterministic models developed so far are modifications of the Streeter-Phelps equations to take into account the principal factors (photosynthesis and respiration, benthal demand, temperature, etc.) affecting stream quality.

Stochastic models deal with processes which have statistical behavior or statistical inputs, and more nearly represent the physical situation in a river stream. The effect of the stochastic changes on the water quality variables and parameters have been studied with varying levels of sophistication. Thayer and Krutchkoff (1966) developed a stochastic model. The mean BOD and DO values predicted by this model were compatible with those of Dobbins' (1964) model. In addition, the model yields probability distributions of BOD and DO concentrations as functions of the time of travel. They proposed to view the problem as a stochastic birth and death process with BOD and DO being changed by small amounts in a very short time interval. The usual assumptions of steady and uniform flow, steady state process, and one-dimensional flow were made.

Custer and Krutchkoff (1969) derived the temporal and spatial probability distributions of BOD and DO resulting from a single source,for an estuary. A non-dispersion model based on Dobbins' (1964) equations with a time varying velocity, and a diffusion model based on O'Connor's (1967) equation were used to derive the probability distributions; Moushegian and Krutchkoff (1969) used a stochastic approach to analyze a series of stream segments of homogeneous conditions. A new segment was considered whenever a major source of pollution was introduced or major changes in stream parameters occurred. The approach was used to generalize the initial conditions not available in Thayer and Krutchkoff (1966). The initial conditions were generalized to permit the output for one stream segment to be the initial conditions for the succeeding stream segment.

Kothandaraman and Ewing (1968) used a deterministic approach but accounted for the stochastic variations in the reaction velocity constants by using Monte Carlo simulation. The photosynthesis term was included in their model as a periodic function. Recently, Lee and Sims (1972) described an application of stochastic control theory to the dynamic management of control of water pollution in a stream. They simulated stream conditions by assuming that the process had a statistical input while the state equations were deterministic. The modified Streeter-Phelps model was employed and the disturbances assumed to be a white Gaussian process.

2.3 PARAMETER ESTIMATION IN WATER QUALITY

The mathematical models developed so far represent an attempt to duplicate the natural processes that regulate water quality. In most of the cases, a considerable knowledge of the nature of the river system may be available from the basic physics or chemistry of the process taking place in the stream. However, the specific values of the water quality parameters may be unknown. Therefore, the problem of estimation of parameters in water quality models must be considered. In general, some of the BOD and DO parameters have been determined by laboratory tests of water samples or graphical techniques (O'Connel and Thomas, 1965; Davidson and Bradshaw, 1967; O'Connor and DiToro, 1970). Shastry et al. (1973) used available nonlinear techniques (Bard's method) to estimate parameters in several differential models (plug flow models under steady state conditions). Two of these models include nonlinear kinetic mechanisms for BOD decay. One of the models was linear in BOD and DO. The least squares and maximum likelihood functions were used as the criterion functions for estimation. The computational procedure was very involved since numerical integration of the differential equations was required for every iteration of the identification procedure.

In many instances the estimation of parameters in a dynamical model can be reduced to the simpler problem of estimating parameters in an algebraic model. Koivo and Phillips (1972) estimated the BOD concentration, the BOD removal coefficient and the photosynthesis minus respiration term from DO measurements. The analytical solution of a modified Streeter-Phelps model under steady state conditions was used. The procedure provides a least squares fit to the DO measurements and can be incorporated for on-line use, but it is applicable only to linear models. However, as the number of parameters to be determined increased, the number of monitoring stations had to be increased. Marske and Polkowski (1972) use the analytical solution of the monomolecular kinetic model to estimate the rate constant of the BOD reaction and the ultimate BOD from actual data. Several methods of estimation were employed: the Reed and Theriault method, the method of moments, the Thomas-slope method and the Gauss method. The sum of squares surface was used to investigate the quality of the methods. The Gauss method was found to give the best estimates of the parameters.

The models used in the investigations presented above give rise to lumped parameter system identification problems. Such identification problems are easy to solve when an analytical solution is available (linear systems) but becomes more involved if the ordinary differential equations are to be integrated before the estimation of parameters can be done. The problem of identification of parameters in distributed parameter systems (e.g., time varying models), has not been pursued in detail in water quality modeling, although it has been widely studied in other areas. A review of this work has been presented by Lizcano et al. (1973). The only work that has appeared so far, is the one by Koivo and Phillips (1971). They were concerned with the identification of parameters in time varying models from noisy BOD and DO data. No stochastic inputs were used in their system. The least squares function was used as the criterion function for estimation and a stochastic algorithm of the Robbins-Munro type was applied to estimate some of the parameters. It was noted that at least three data locations were needed to construct the algorithm.

2.4 SPECTRAL ANALYSIS

In developing any water pollution program it is necessary to obtain water quality data. This type of data can be classified as stochastic in nature. Spectral analysis is a powerful technique to analyze this type of data. Results obtained from spectral analysis are often used for model building and prediction purposes.

Several investigators (Wastler, 1963; Gunnerson, 1966; Thomann, 1967, 1969; Fan et al., 1970; Shastry et al., 1972) have applied spectral analysis to specific problems in water quality management. Wastler (1963) described a method which calculates the individual power spectra of a given time series. Physical interpretation of each of the harmonics present at different stations was attempted in light of the advective and diffusive processes, the diurnal variations of the waste discharge and the photosynthetic activity. Gunnerson (1966), treated the problem of optimizing sampling time interval for water quality measurements. He concluded that each environment has peculiar data collection requirements. Thomann (1967, 1969) analyzed DO and temperature data from the Delaware River. He divided the harmonics present in the record into low and high frequency harmonics. The low frequency harmonics were attributed to variations of the DO saturation value and the photosynthesis term with temperature, estuarine flow and the microbial growth process. Diurnal variations of DO and temperature were included in the high frequency harmonics. Fan et al. (1970) and Shastry et al. (1972) calculated and interpreted individual power spectra of several water quality variables using data from Ohio River monitoring stations. In addition, the technique of cross-spectral analysis was introduced. Models for water quality were developed by using the results of spectral analysis as well as other available information.

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LIST OF SYMBOLS

Symbol	Definition
i	Denotes properties in the i-th stream section
k_0	Saturation constant
k_1	Bacterial action constant
k_1'	Coefficient of carbonaceous oxidation
k_1''	Coefficient of nitrogenous oxidation
k_2	Reaeration constant
k_3	Rate constant for BOD sedimentation
q	Net river flow
r	Width of the stream
t	Time
t_s	Time lag
x	Distance downstream from reference $x = 0$
x_o	Point of outfall of waste along the stream
A	Cross-sectional area
C	DO concentration
C_p	Specific heat of water in the stream
C_s	Saturation level for oxygen concentration
D_B	DO depletion due to benthal demand
D_L	Longitudinal dispersion rate coefficient

K	Temperature dissipation
K_L	Saturation constant
L	BOD concentration
L_a	BOD addition due to local runoff
L'_x	Carbonaceous BOD concentration
N_x	Distribution of nitrogenous BOD concentration
P	Algal photosynthetic oxygen source
R	Algal respiration sink
T	Water temperature
T_e	Equilibrium water temperature
U	Stream velocity
U_o	Initial stream velocity at some point of waste discharge
ρ	Density of water in stream
τ	Time of travel
$\Sigma_{L,C}$	Sources and sinks of BOD and DO, respectively

CHAPTER 3

IDENTIFICATION OF PARAMETERS IN TRANSIENT MODELS FROM STOCHASTIC WATER QUALITY DATA

3.1 INTRODUCTION

The quality of water of polluted streams has often been described by steady state models in the form of ordinary differential equations (Streeter and Phelps, 1925; Dobbins, 1964). These models are not adequate to simulate actual conditions in streams when substantial changes in stream quality take place over a period of operation. These changes may be investigated by using a model which describes water quality variations as a function of time and distance (Dresnack and Dobbins, 1968). This model is generally represented by partial differential equations.

Although time-varying or transient models produce continuous estimates of river conditions they may not represent the exact variations of stream characteristics. This is because they do not take into account the random variations in stream conditions and local environmental conditions. It may be possible to account for these variations by adding a stochastic component, such as white noise, to the model equations.

In order to use the model equations for predicting the temporal and spatial variations of stream quality, it is necessary to determine the various parameters that appear in the models. The problem of determining these parameters reduces to one of estimating parameters in partial differential equations. This is a well-known problem in process identification and has been studied by many investigators (Seinfeld and Chen, 1971; Malpani and Donnelly, 1972) in several fields of engineering. To the author's knowledge only one paper (Koivo and Phillips, 1971) has been reported in the literature on estimation of parameters in water quality models described by partial differential equations. The investigation concerned identification of parameters from noisy BOD and DO data. Using the least squares techniques, a stochastic algorithm was applied to estimate some of the parameters appearing in the model equations. At least three data locations were needed to collect data for parameter estimation.

The most time-consuming computational step in most of the methods for parameter estimation in partial differential equations is the integration of the model equations which must be done for each iteration of the parameter estimation procedure. This integration step can be avoided if an analytical solution exists for the model equations. On the other hand, the number of data locations is an important factor in collecting data for parameter estimation. Therefore, it is highly desirable to select parameter estimation procedures in which number of data points needed and the number of data locations employed are minimum.

The purpose of this chapter is to show that the parameters appearing in the model equations may be estimated from experimental data on BOD and DO collected at as few as two locations using a minimum of data points. The experimental data used for parameter estimation are made up of a deterministic component and a stochastic component. Because of variations in environmental conditions, a random component has been added to account for the stochastic variations in stream quality at the beginning of the river section considered

3.2 MATHEMATICAL MODEL

In this work the plug flow model is used to represent the temporal and spatial distribution of BOD and DO concentrations, assuming isothermal conditions. In addition, the following mechanisms are taken into account:

1. The decrease in the oxygen concentration due to bacterial oxidation which is proportional to the BOD present (it obeys a first order rate),
2. the decrease in the BOD concentration by sedimentation,
3. the addition in the BOD concentration by local runoff,
4. the increase in the DO concentration due to reaeration from the atmosphere,
5. the removal of oxygen by the respiration of plankton and fixed plants,
6. the increase of oxygen by photosynthetic action of plankton and fixed plants.

Under these assumptions the system equations describing the spatial and temporal distribution of BOD and DO can be written as

$$\frac{\partial L}{\partial t} + u\frac{\partial L}{\partial x} + (k_1 + k_3)L - L_a = 0 \tag{3.1}$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + k_1 L - k_2(C_s - C) - \langle P - R \rangle = 0 \tag{3.2}$$

where

k_1 = bacterial action constant

k_2 = reaeration constant

k_3 = rate constant for BOD sedimentation

t = time

u = stream velocity

x = distance downstream from the reference point ($x = 0$)

C = DO concentration as a function of t and x

C_s = saturation level for oxygen concentration

L = BOD concentration as a function of t and x

L_a = BOD addition rate due to local runoff

$\langle P - R \rangle$ = rate of the algal photosynthesis minus rate of respiration

The initial condition is given by

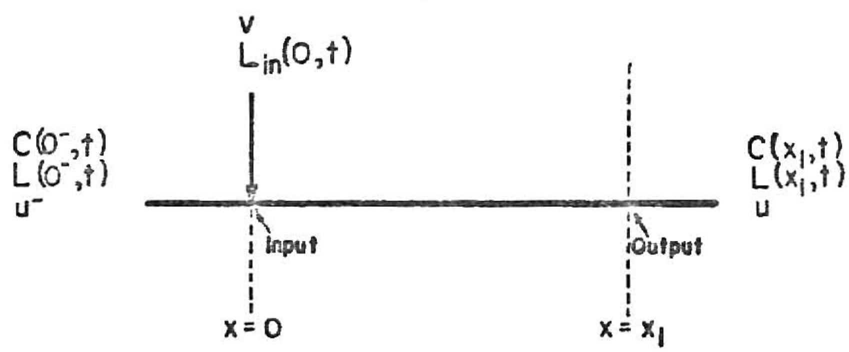
$$t = 0, \qquad \frac{\partial L}{\partial t} = \frac{\partial C}{\partial t} = 0 \tag{3.3}$$

and the boundary conditions by

$$x = 0^+, \quad L = L_o, \quad C = C_o, \quad t < 0 \tag{3.4a}$$

$$x = 0^+, \quad L = L(t), \quad C = C(t), \quad t \geq 0 \tag{3.4b}$$

Equation (3.3) indicates that initially ($t = 0$) the BOD and DO profiles are at the steady state condition. The boundary condition (3.4a) is needed to determine the steady state profiles. At $t = 0$, there is a waste discharge into the stream at $x = 0$ which disturbs the system. Assuming instantaneous mixing of the waste with the stream flow, the conditions of water quality immediately following the mixing point (see Fig. 3.1) can be represented by equation (3.4b). Equations (3.1) and (3.2) constitute a set of partial differential equations which represent a linear distributed parameter system. This set of partial differential equations can be solved by using the Laplace transformation (DiToro and O'Connor, 1968), the method of characteristics (DiToro, 1969; Koivo and Phillips, 1971) or finite differences (Malpani and Donnelly, 1972).



$$u \equiv u^- + v$$

$$L(0,t) = \frac{u^-}{u} L(0,t) + \frac{v}{u} L_{in}(0,t)$$

$$C(0,t) = C(0^-,t)$$

Fig. 3.1 Sketch of a stream affected by a waste discharge

The method of characteristics is employed in this investigation to solve equations (3.1) and (3.2). The application of this method permits the transformation of the set of PDE into a set of ordinary differential equations which can be integrated numerically with precision when no analytical solution is available. Details concerning the method of characteristics and its application in solving the system equations are given in Appendices 3.1 and 3.2 respectively.

The direct application of the method of characteristics yields (see Abbot, 1966)

$$\frac{dx}{dt} = u \tag{3.5}$$

$$\frac{dL}{dt} = -(k_1 + k_3)L + L_a \tag{3.6}$$

$$\frac{dC}{dt} = - k_1 L + k_2 (C_s - C) + \langle P - R \rangle \tag{3.7}$$

Equation (3.5) represents the characteristic lines along which equations (3.6) and (3.7) can be integrated. The solution to these equations may be divided into two parts depending upon whether the boundary conditions are chosen along the x = 0 or the t = 0 axes. The solution obtained by using the boundary conditions along the t = 0 axis ($0 \leq t \leq x/u$) represents the initial steady state for various positions ($x \geq ut$). The solution obtained when using the boundary conditions along the x = 0 axis ($t \geq x/u$) represents the response of the system to the waste input at various positions ($0 \leq x \leq ut$) as a function of time.

For the system shown in Fig. 3.1, the solution reeuces to (see Appendix 3.2)

1. for $0 \leq t \leq x/u$ (initial condition along the $t = 0$ axis; $x \geq ut$)

$$L(x,t) = L(x - ut, 0)e^{-(k_1 + k_3)t} + \frac{L_a}{k_1 + k_3}[1 - e^{-(k_1 + k_3)t}] \tag{3.8}$$

$$C(x,t) = C_s[1 - e^{-k_2 t}] - \frac{k_1[L(x - ut, 0) - \frac{L_a}{k_1 + k_3}]}{k_2 - (k_1 + k_3)}[e^{-(k_1 + k_3)t} - e^{-k_2 t}]$$
$$+ \frac{1}{k_2}[\langle P - R\rangle - \frac{L_a}{k_1 + k_3}][1 - e^{-k_2 t}] + C(x - ut, 0)e^{-k_2 t} \tag{3.9}$$

2. for $t \geq x/u$ (Initial condition along the $x = 0$ axis; $0 \leq x \leq ut$)

$$L(x,t) = L(0^+, t - x/u)e^{-(k_1 + k_3)x/u} + \frac{L_a}{k_1 + k_3}[1 - e^{-(k_1 + k_3)x/u}] \tag{3.10}$$

$$C(x,t) = C_s[1 - e^{-k_2 x/u}] - \frac{k_1[L(0^+, t - x/u) - \frac{L_a}{k_1 + k_3}]}{k_2 - (k_1 + k_3)}[e^{-(k_1 + k_3)x/u}$$
$$- e^{-k_2 x/u}] + \frac{1}{k_2}[\langle P - R\rangle - \frac{L_a}{k_1 + k_3}][1 - e^{-k_2 x/u}]$$
$$+ C(0^+, t - x/u)e^{-k_2 x/u} \tag{3.11}$$

where $L(0^+, t - x/u)$ and $C(0^+, t - x/u)$ are the BOD and DO concentrations at $x = 0^+$, respectively, after the mixing of waste with the stream flow. These values may be represented by any function of time. Equations (3.10) and

(3.11) reduce to the known steady state solutions (Camp, 1963) when the BOD and DO concentrations at $x = 0^+$ are not time dependent. Equations (3.8) to (3.11) may be generalized to consider a stream affected by multiple discharges (see Appendix 3.3).

It is worth noting in equations (3.10) and (3.11) that if BOD and DO values measured at two locations (say at $x = 0^+$ and $x = x_1$) are correlated in the time domain, it may be found that

1. There exists a positive correlation between downstream BOD values ($x = x_1$) and BOD values at $x = 0^+$. A strong correlation would be found at a lag $\tau = x_1/u$.

2. There exists a positive correlation between downstream DO values and DO values at $x = 0^+$, and a negative correlation between downstream DO values and BOD values at $x = 0^+$. Downstream DO values are also negatively correlated with downstream BOD values. Again, strong correlations would be found at a lag $\tau = x_1/u$. Similar conclusions were obtained by Shastry et al. (1972) by appling spectral analysis techniques to actual data from several rivers. This lag represents the time a slug of material takes on going from $x = 0^+$ to the end of the section at $x = x_1$. It is the pure time delay of the system. This implies that information about the system at $x = x_1$ is not available until after a finite time lag. This time lag phenomenon may be used to correlate BOD and DO values measured at $x = 0^+$ with BOD and DO values measured at $x = x_1$, and the correlation equations [equations (3.10) and (3.11)] used to estimate the parameters that appear in the model equation. Therefore, only two monitoring stations are needed to collect data for parameter estimation.

3.3 FORMULATION OF THE PROBLEM

The stream section considered in this study is portrayed in Fig. 3.1. The data obtained from the monitoring facility at the beginning of the section ($x = 0^+$) is referred to as input data, and the response to the input measured at the end of the section at $x = x_1$ is considered as the output data.

It is assumed that BOD and DO variations at the beginning of the section just below the waste discharge ($x = 0^+$, see Fig. 3.1) are made up of a deterministic component and a stochastic component. Two representations of the deterministic component are used: a step function and a sine function. The stochastic component is assumed to be normally distributed with a mean of zero and a finite standard deviation of σ [$N(0, \sigma)$]. The stochastic component represents the random variations in stream quality due to changes in environmental conditions.

In order to correlate BOD and DO values obtained at $x = 0^+$ with values obtained at $x = x_1$, the value of $\tau = x_1/u$ needs to be known with some approximation. The value of x_1 can be determined without excessive error but u is generally not accurately known. Because of this uncertainty in the value of u, we may choose to consider τ as a parameter together with k_1, k_2, k_3, L_a, and $\langle P-R \rangle$. An initial estimate of τ that is to be used in the parameter identification procedure can be obtained by estimating an approximate value for u either from experimental measurements or from empirical correlations. Furthermore, it is likely that the initial estimate of τ may be a good esimate of the true value. In this case τ need not be considered as an additional parameter.

Four cases are considered in this work. The first two involve the use of equation (3.10) and the others the use of equation (3.11). They are defined in Table 3.1. Columns (1) - (4) list the case numbers, the boundary conditions (at $x = 0^+$, after mixing), the parameters assumed to be known, and the parameters to be estimated, respectively. The period of the sine wave to be used is 365 days which represents yearly variations in actual records.

3.4 COMPUTATIONAL ALGORITHM AND PROCEDURE

Let us assume that the parameters appearing in equations (3.8) - (3.11) are constant for a section with a fixed length x_1. Let us also assume that the estimation procedure starts after $t = 0$. To correlate input-output data only equations (3.10) and (3.11) are needed. It can be observed that equation (3.10) may be represented by a straight line when $L(x_1, t)$ (the dependent or output variable) is plotted versus $L(0^+, t - x_1/u)$ (the independent or input variable). The slope of such a line should be $\exp[-(k_1 + k_3)x_1/u]$. The interception of the line with the $L(x_1, t)$ axis is given by the second term in the right hand side of equation (3.10) (see Fig. 3.2). Similarly, equation (3.11) may be represented by a surface on the tridimensional coordinate space formed by $C(x_1, t)$, $C(0^+, t - x_1/u)$, and $L(0^+, t - x_1/u)$. This surface represents a plane (see Fig. 3.3).

For all the four cases (Cases 1 - 4) the least square criterion function can be used to fit the data. Cases 1 and 2 will give a straight line fit (see Fig. 3.2), whereas Cases 3 and 4 will result in a plane (see Fig. 3.3). However, for simplicity, Cases 3 and 4 can also be fitted by a straight line if it is assumed that $L(0^+, t - x_1/u)$ is constant with respect to time in equation (3.11), i.e., $L(0^+, t) = L_i$.

Table 3.1 Conditions for Parameter Estimation

Case (1)	Boundary Conditions at $x = 0^+$, after mixing (2)	Assumptions (3)	Parameters to be Identified (4)
1	BOD is made up of a constant value (step function) and a normal distributed random variable	La is known	k_r, τ
2	BOD is made up of a cyclic component (sine) and a normal distributed random variable	La is known	k_r, τ
3	BOD is given by a single value, DO is made up of a constant value (step function) and a normal distributed random variable	C_s and τ are known	k_1, k_2, k_3, La <P-R>, $L(0, t) = L_A$
4	BOD is given by a single value, DO is made up of a cyclic component (sine) a normal distributed random variable	C_s and τ are known	k_1, k_2, k_3, La <P-R>, $L(0^+, t) = L_A$

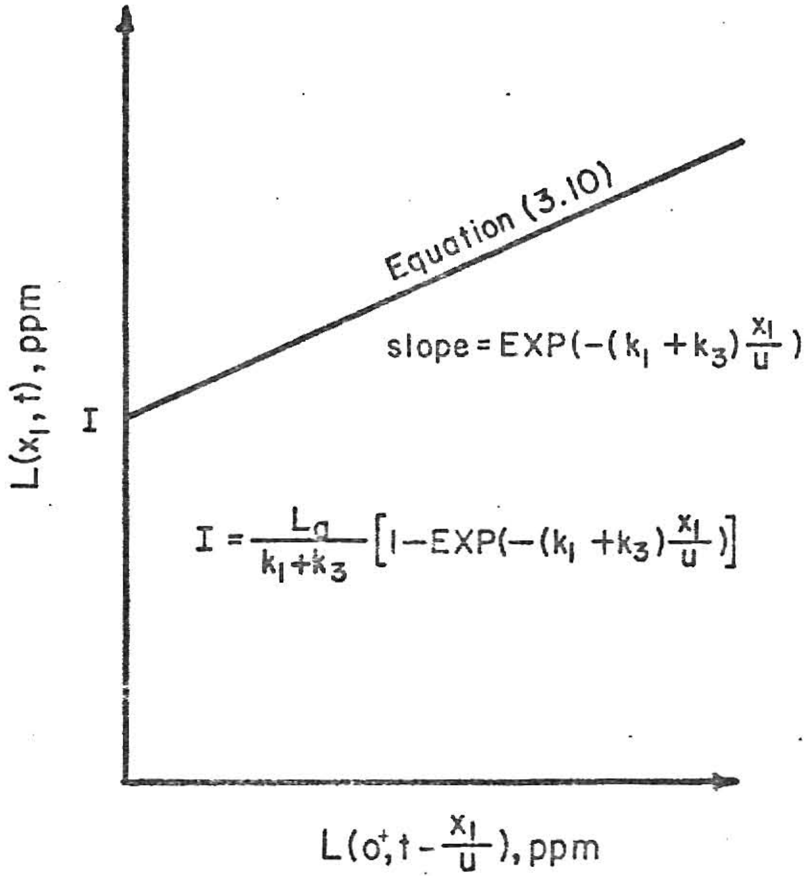


Fig. 3.2 Graphical representation of the relationship between BOD concentrations at two locations.

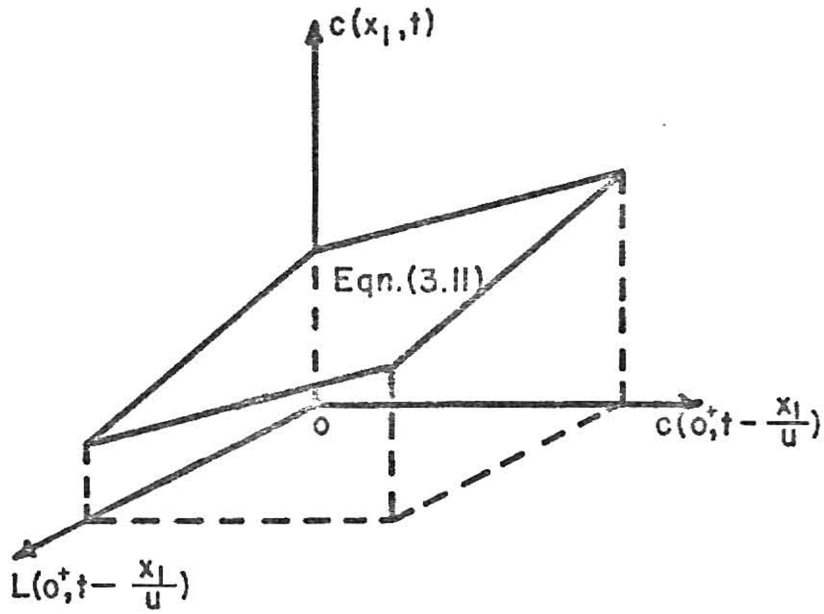


Fig. 3.3 Graphical representation of the relationships between DO concentrations and BOD concentrations at two locations.

Equations (3.10) and (3.11) can be represented in general in the form of a relationship between the independent (input) and the dependent (output) variables as shown below.

$$y_j = f(\underline{x}_j, \underline{\theta}) + \varepsilon , \qquad j = 1, 2, \ldots, n. \tag{3.12}$$

where

y_j = measured dependent (output) variable for the j-th experiment

$\underline{x}_j$ = vector of independent (input) variables, $(x_{1j}, \ldots, x_{mj})$

$\underline{\theta}$ = vector of parameters to be estimated, $(\underline{\theta}_1, \ldots, \underline{\theta}_k)$

ε = experimental error

Equation (3.12) is said to be linear in the parameters if it can be converted to a model of the form

$$y = \underline{\theta}_1 + \underline{\theta}_2 z_1 + \underline{\theta}_3 z_2 + \ldots + \underline{\theta}_k z_{k-1} \tag{3.13}$$

where

z_i = functions of the independent variables $\underline{x}$

Any mathematical model which cannot be converted to this form is considered a nonlinear model with respect to the parameters. The estimation of parameters for nonlinear models is not straightforward and generally more involved and requires the use of nonlinear optimization techniques.

The parameters for nonlinear models are, usually, determined by minimizing a selected criterion function, S, which is a measure of the difference between the observed (measured) and predicted values of the dependent variables. The independent variables are assumed to be accurately known. The selected criterion function in this study is the sum of squares criterion function, and it is of the form

$$\min_{\{\underline{\theta}\}} S(\underline{\theta}) = \min_{\{\underline{\theta}\}} \sum_{j=1}^{n} [y_j - f(\underline{x}_j, \underline{\theta})]^2 \tag{3.14}$$

Many methods exist for effecting this type of optimization. The Gauss-Newton method with modifications by Carrol (1961), Eisenpress and Greensdadt (1966), and Bard (1967) can be used to estimate the parameters in equations (3.10) and (3.11). This method is frequently refered to as Bard's method and a brief description of it is given in Appendix 3.4.

For the section of the stream shown in Fig. 3.1, the parameters in the model equations, equations (3.10) and (3.11), were estimated using simulated data on BOD and DO and the computational algorithm developed in the preceding paragraphs. At each monitoring facility ($x = 0^+$ and $x = x_1$), a total of 30 data points were obtained. The BOD and DO variations at $x = 0^+$ (input) were made up of a deterministic component and a stochastic component. Four cases were considered. In Cases 1 and 3, the deterministic component was represented by a step function, whereas in Cases 2 and 4, the deterministic component was a sine function. Values of the stochastic component for all the four cases were normally distributed with a mean of zero and a finite standard deviation of σ. These normally distributed random variates were generate on the digital computer using the IBM scientific subroutine GAUSS (IBM, 1966). Four different values of σ, viz., 10^{-4}, 10^{-3}, 10^{-2} and 10^{-1} ppm were chosen to examine the effect of the spread in the data used for parameter estimation. The parameter values and the mathematical expressions used in the simulation are summarized in Tables 3.2 and 3.3, respectively.

Table 3.2 Typical Set of Parameters Used for Cases 1 through 4*

Parameter	Case	Value	
k_1	1 through 4	0.160	1/day
k_2	3 and 4	0.710	1/day
k_3	1 through 4	0.200	1/day
$\langle P-R \rangle$	3 and 4	0.125×10^1	ppm/day
La	1 through 4	0.200	ppm/day
$L(0^+, t) = L_A$	3 and 4	0.200×10^2	ppm
C_s	3 and 4	0.860×10^1	ppm
$\tau = x_1/u$	1 through 4	0.100×10^1	day

*Some of these parameters have been obtained from Fan et al. (1972)

Table 3.3 Expressions Used to Generate the Data for Cases 1 to 4

Case (1)	Conditions at $x = 0^+$ (2)	Conditions at $x = x_1$ (3)
1	$L(0^+,t) = 20.0 + N(0,\sigma)$	$L(x_1,t)$ = given by equation (3.10)
2	$L(0^+,t) = 15.0 + 5.0 \sin(2\pi t/365) + N(0,\sigma)$	$L(x_1,t)$ = given by equation (3.10)
3	$C(0^+,t) = 7.0 + N(0,\sigma)$	$C(x_1,t)$ = given by equation (3.11)
4	$C(0^+,t) = 7.0 + \sin(2\pi t/365) + N(0,\sigma)$	$C(x_1,t)$ = given by equation (3.12)

It can be observed in equation (3.10) that k_1 and k_3 appear combined as $(k_1 + k_3)$. When only BOD data is used for parameter estimation, k_1 could not be estimated independently of k_3. This can be explained as follows. Let us assume, for example, that the expression $(k_1 + k_3)$ is equal to 0.36. It is obvious that many pairs of k_1 and k_3 values could give the same sum of 0.36. Because of this, the expression $(k_1 + k_3)$ must be estimated as a single parameter in Cases 1 and 2, i.e., $k_r = (k_1 + k_3)$.

In all four cases, Bard's method was used to determine the parameter estimates. In Cases 1 and 2, the initial estimates of k_r and τ were chosen arbitrarily. These initial estimates were then used in equation (3.10) in conjunction with the input BOD data to predict the output BOD values. The difference between the measured output and the predicted output was used to improve the initial estimates of k_r and τ. The procedure was repeated until further iteration resulted in no significant change in k_r and τ.

A similar procedure was followed in Case 3 to estimate the parameters except that the input DO data and the corresponding DO equation (3.11) were used instead of BOD data and equation (3.10). The parameter estimated in Case 3 were k_1, k_2, k_3, $\langle P\text{-}R \rangle$, L_a and $L(0, t)$, i.e., L_A. Case 4 was divided into two parts, viz., Cases 4A and 4B. The procedure for estimating the parameters in both cases was essentially the same as that used in Case 3. In Case 4A, the actual or nominal values of the parameters were used as the initial estimates whereas in Case 4B, the initial estimates were arbitrarily chosen. This was done to compare the extent of the error induced in the selection of the initial estimates.

An IBM 360/50 Digital Computer was used to perform the simulation and calculations. The programs were written in Fortan IV programming language.

3.5 RESULTS

Cases 1 and 2 differ in the definition of the deterministic component at $x = 0^+$. Numerical results of the parameters obtained for these cases are presented in Tables 3.4 through 3.7 for different values of σ. Column (1) in all the tables shows the estimated parameters. For Case 1, Columns (2) and (3), respectively, show the initial guesses for the iterative procedure, the final estimates of the parameters, and the standard deviation of the parameters. Similarly, for Case 2, Columns (5), (6) and (7) show, respectively, the initial guesses for the iterative procedure, the final estimates of the parameters, and the standard deviation of the parameters. Graphical results for both cases are presented in Figs. 3.4 through 3.6. In these figures, Case 1 is represented by a rhombus, Case 2 is represented by a circle and the actual value of the parameters by a solid line. Figure 3.4 shows the deviations of k_r from its actual value as a function of σ. Similarly, Fig. 3.5 shows the deviations of τ from its actual value as a function of σ. Figure 3.6 shows the minimized least squares criterion function S [see equation (3.14)] as a function of σ, for Cases 1 and 2.

Tables 3.8 through 3.11 show the numerical results of the parameters obtained for Case 3 and Tables 3.12 through 3.15 the numerical results of the parameters for Cases 4A and 4B. Figures 3.7 through 3.12 show the deviation of the various parameters, such as k_1, k_2, k_3, $\langle P\text{-}R\rangle$, L_a and $L(0, t) = L_A$, from their actual values as functions of σ. In these figures, the square symbols represent the parameter estimates for Case 3, the plus symbols represent the parameter estimates for Case 4A and the cross symbols

Table 3.4 Estimated Values of Parameters Using the BOD Equation for $\sigma = 10^{-4}$

Parameter (1)	Case 1 Initial Guesses (2)	Case 1 Final Estimates (3)	Case 1 Standard Deviation (4)	Case 2 Initial Guesses (5)	Case 2 Final Estimates (6)	Case 2 Standard Deviation (7)
k_r	0.420	0.267814	0.6524×10^{-5}	0.300	0.359991	0.0
τ	0.15×10^{1}	0.136030×10^{1}	0.3469×10^{-4}	0.110×10^{1}	0.100001×10^{1}	0.0

Table 3.5 Estimated Values of Parameters Using the BOD Equation for $\sigma = 10^{-3}$

	Case 1			Case 2		
Parameter (1)	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)	Initial Guesses (5)	Final Estimates (6)	Standard Deviation (7)
k_r	0.300	0.210594	0.1803×10^{-3}	0.340	0.359996	0.1274×10^{-5}
τ	0.900	0.175229×10^{1}	0.1590×10^{-2}	0.900	0.999996	0.3690×10^{-5}

Table 3.6 Estimated Values of Parameters Using the BOD Equation for $\sigma = 10^{-2}$

	Case 1			Case 2		
Parameter (1)	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)	Initial Guesses (5)	Final Estimates (6)	Standard Deviation (7)
k_r	0.330	0.284449	0.2263×10^{-2}	0.380	0.359991	0.7173×10^{-5}
τ	0.800	0.127721×10^{1}	0.1061×10^{-1}	0.120×10^{1}	0.100001×10^{1}	0.2077×10^{-4}

Table 3.7 Estimated Values of Parameters Using the BOD Equation for $\sigma = 10^{-1}$

Parameter (1)	Case 1			Case 2		
	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)	Initial Guesses (5)	Final Estimates (6)	Standard Deviation (7)
k_r	0.310	0.269474	0.5951×10^{-2}	0.400	0.359992	0.0
τ	0.700	0.135149×10^{1}	0.3123×10^{-1}	0.140×10^{1}	0.100001×10^{1}	0.0

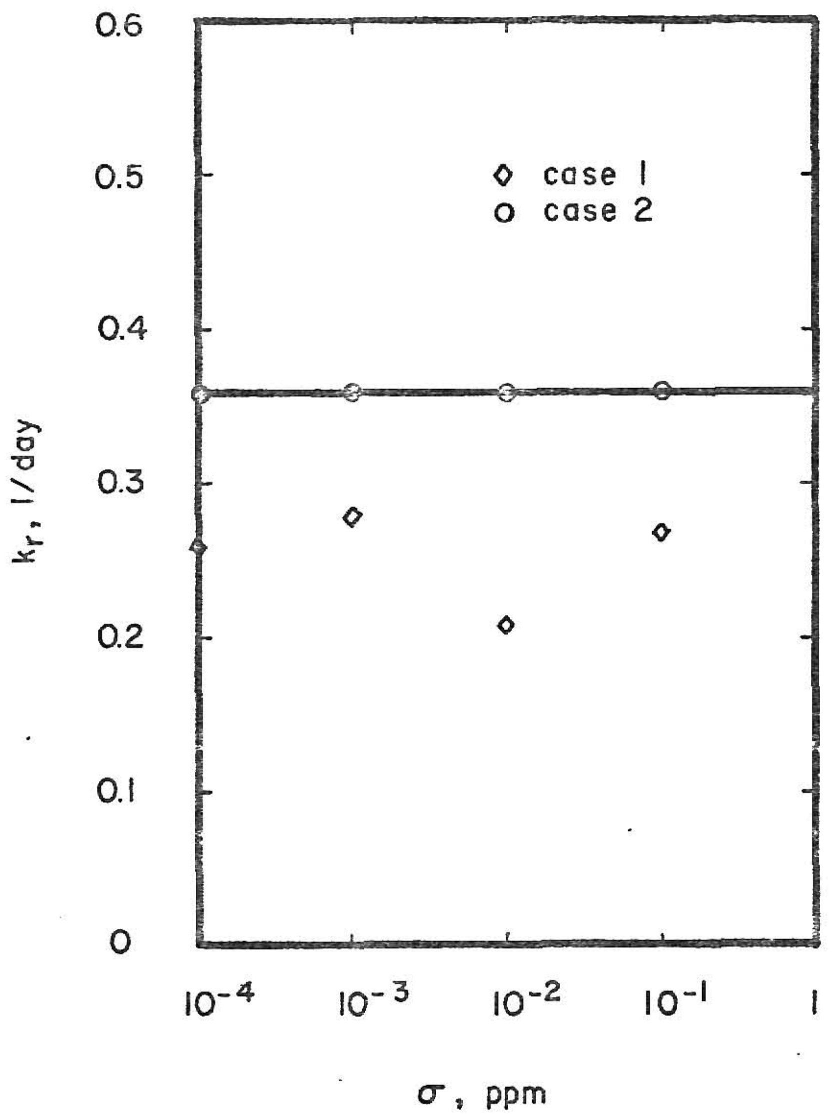


Fig. 3.4 Estimated values of k_r as a function of σ for cases 1 and 2

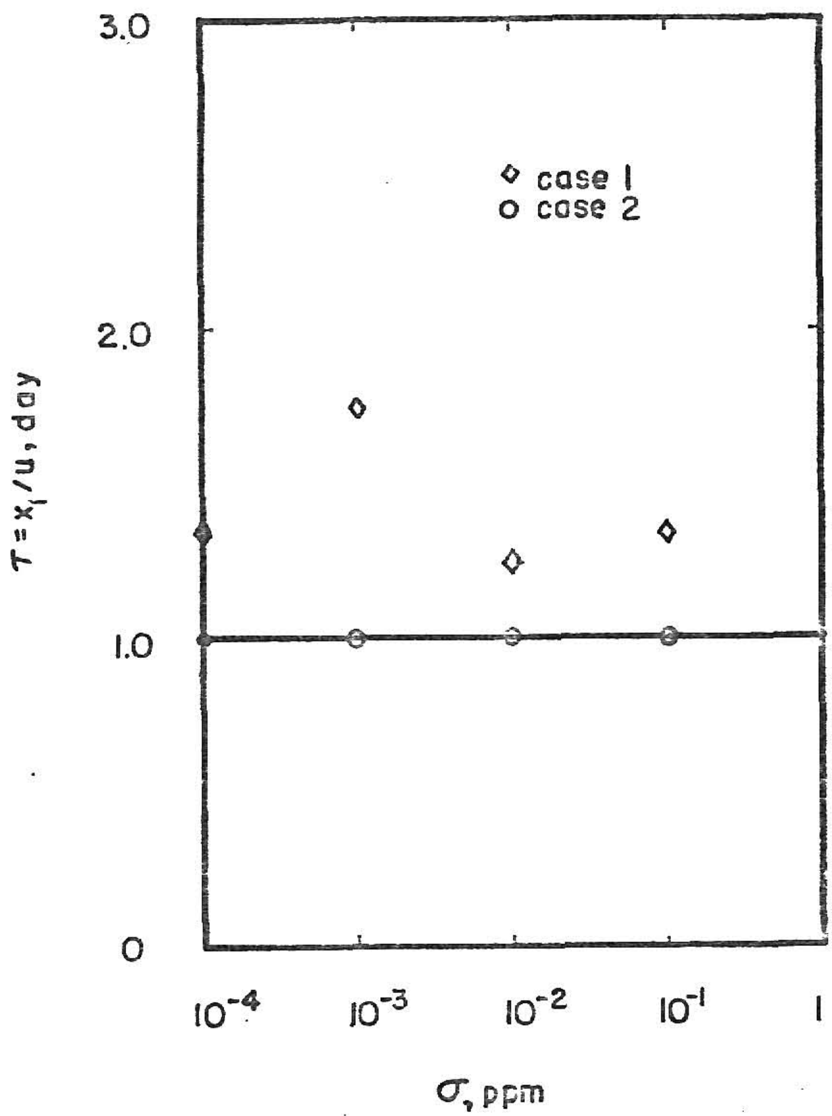


Fig. 3.5 Estimated values of τ as a function of σ for Cases 1 and 2

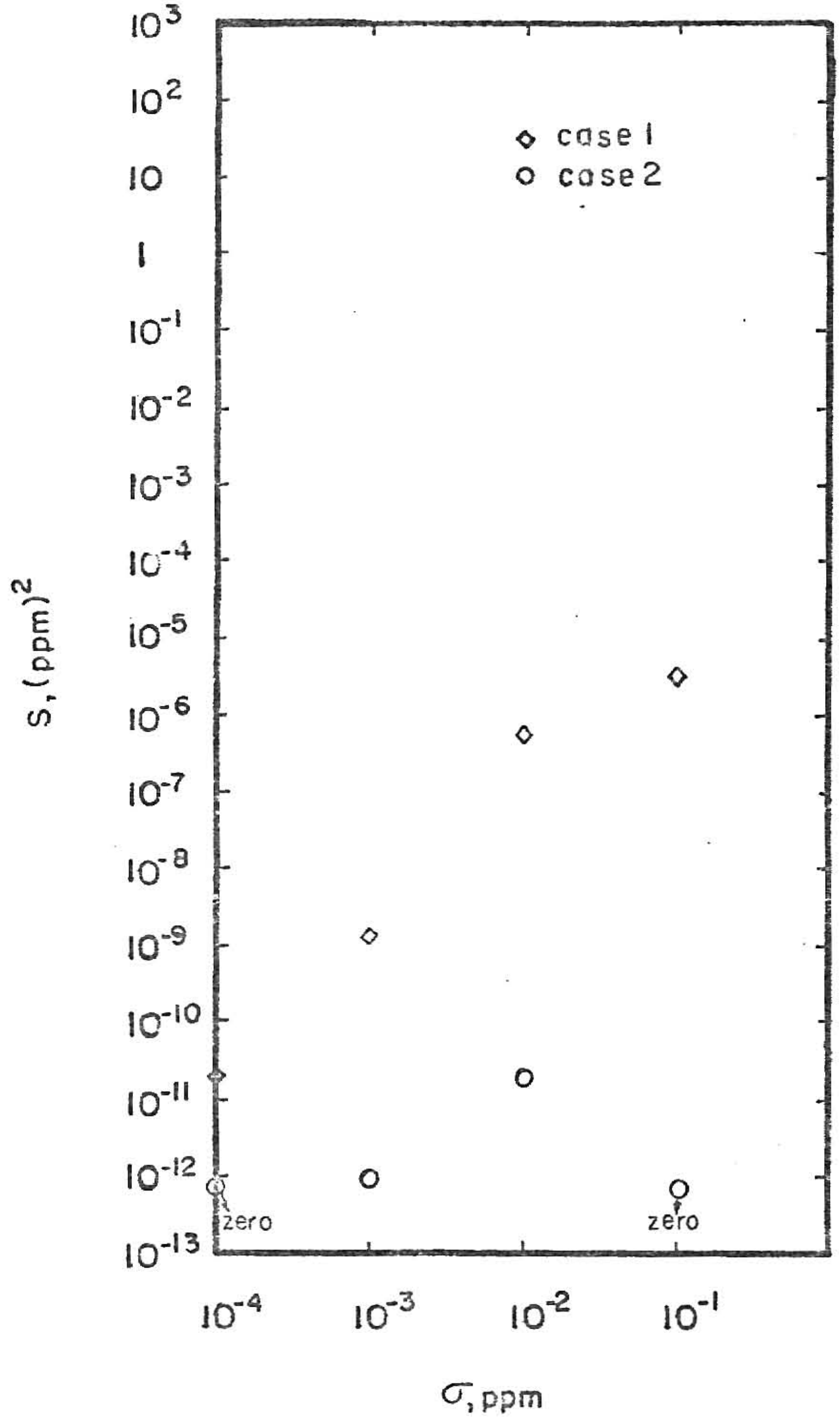


Fig.3.6 Estimated values of S as a function of σ for Cases 1 and 2

Table 3.8 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.0001$

Case 3

Parameter (1)	Case 3: Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)
k_1	0.170	0.167875	0.9012×10^{-2}
k_2	0.700	0.690874	0.1371
k_3	0.210	0.209196	0.1498×10^{-1}
<P-R>	0.130×10^{1}	0.128597×10^{1}	0.1247
La	0.170	0.519251	0.4723×10^{1}
L(0,t)	0.190×10^{2}	0.190523×10^{2}	0.3793

Table 3.9 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.001$

Case 3

Parameter (1)	Case 3: Initial Guesses (2)	Case 3: Final Estimates (3)	Case 3: Standard Deviation (4)
k_1	0.110	0.135689	0.1585
k_2	0.750	0.818369	0.1835×10^1
k_3	0.190	0.208580	0.1082
<P-R>	0.100×10^1	0.172207×10^1	0.1382×10^1
La	0.240	0.135870×10^1	0.1964×10^2
L(0,t)	0.220×10^2	0.287233×10^2	0.1234×10^2

Table 3.10 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.01$

Case 3

	Case 3		
Parameter (1)	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)
k_1	0.170	0.218634	0.4609
k_2	0.730	0.874225	0.1076×10^1
k_3	0.250	0.254081	0.6320
$\langle P-R \rangle$	0.140×10^1	0.275742×10^1	0.5856×10^1
La	0.230	0.389749	0.3210×10^2
L(0,t)	0.240×10^2	0.259759×10^2	0.1880×10^2

Table 3.11 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.1$

Case 3

	Case 3		
Parameter (1)	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)
k_1	0.120	0.106216	0.2930×10^{-4}
k_2	0.650	0.710009	0.9224×10^{-5}
k_3	0.180	0.208204	0.3634×10^{-4}
<P-R>	0.110×10^{1}	0.146445×10^{1}	0.4061×10^{-3}
La	0.170	0.288424×10^{1}	0.1524×10^{-1}
L(0,t)	0.180×10^{2}	0.302619×10^{2}	0.3291×10^{-2}

Table 3.12 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.0001$

	Case 4A			Case 4B		
Parameter (1)	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)	Initial Guesses (5)	Final Estimates (6)	Standard Deviation (7)
k_1	0.160	0.159995	0.1027×10^{-4}	0.170	0.160530	0.2732×10^{-4}
k_2	0.710	0.710007	0.1594×10^{-5}	0.700	0.710010	0.1672×10^{-5}
k_3	0.200	0.200005	0.9277×10^{-5}	0.210	0.209430	0.2790×10^{-4}
<P-R>	0.125×10^{1}	0.124999×10^{1}	0.1300×10^{-3}	0.130×10^{1}	0.131588×10^{1}	0.1346×10^{-3}
La	0.200	0.200407	0.2605×10^{-3}	0.170	0.185842×10^{1}	0.1609×10^{-2}
L(0,t)	0.200×10^{2}	0.199995×10^{2}	0.1172×10^{-2}	0.190×10^{2}	0.195417×10^{2}	0.6116×10^{-3}

Table 3.13 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.001$

Parameter (1)	Case 4A Initial Guesses (2)	Case 4A Final Estimates (3)	Case 4A Standard Deviation (4)	Case 4B Initial Guesses (5)	Case 4B Final Estimates (6)	Case 4B Standard Deviation (7)
k_1	0.160	0.160005	0.8151×10^{-4}	0.110	0.130482	0.2206×10^{-3}
k_2	0.710	0.710000	0.1549×10^{-4}	0.750	0.710010	0.3479×10^{-4}
k_3	0.200	0.200008	0.7811×10^{-4}	0.190	0.193947	0.2141×10^{-3}
<P-R>	0.125×10^{1}	0.125011×10^{1}	0.1212×10^{-2}	0.100×10^{1}	0.139577×10^{1}	0.1066×10^{-1}
La	0.200	0.200008	0.1870×10^{-2}	0.240	0.918769	0.3734×10^{-1}
L(0,t)	0.200×10^{2}	0.199994×10^{2}	0.4946×10^{-2}	0.220×10^{2}	0.249946×10^{2}	0.4668×10^{-1}

Table 3.14 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.01$

Parameter (1)	Case 4A Initial Guesses (2)	Case 4A Final Estimates (3)	Case 4A Standard Deviation (4)	Case 4B Initial Guesses (5)	Case 4B Final Estimates (6)	Case 4B Standard Deviation (7)
k_1	0.160	0.160048	0.1229×10^{-4}	0.170	0.181911	0.7354×10^{-1}
k_2	0.710	0.710010	0.1593×10^{-5}	0.730	0.714197	0.7463×10^{-2}
k_3	0.200	0.200015	0.1251×10^{-4}	0.250	0.263433	0.6646×10^{-1}
$\langle P-R \rangle$	0.125×10^{1}	0.125208×10^{1}	0.2217×10^{-3}	0.140×10^{1}	0.198915×10^{1}	0.6022
La	0.200	0.201484	0.1308×10^{-3}	0.230	0.296957	0.7360×10^{1}
L(0,t)	0.200×10^{2}	0.200087×10^{2}	0.5978×10^{-3}	0.240×10^{2}	0.235692×10^{2}	0.3619×10^{1}

Table 3.15 Estimated Values of Parameters Using the DO Equation for $\sigma = 0.1$

	Case 4A			Case 4B		
Parameter (1)	Initial Guesses (2)	Final Estimates (3)	Standard Deviation (4)	Initial Guesses (5)	Final Estimates (6)	Standard Deviation (7)
k_1	0.160	0.160009	0.2997×10^{-3}	0.120	0.936163×10^{-1}	0.1179×10^{2}
k_2	0.710	0.710000	0.3568×10^{-4}	0.650	0.696606	0.6121×10^{1}
k_3	0.200	0.200009	0.2772×10^{-3}	0.180	0.164212	0.1170×10^{2}
<P-R>	0.125×10^{1}	0.125033×10^{1}	0.2768×10^{-2}	0.110×10^{1}	0.841131	0.3875×10^{1}
La	0.200	0.2000047	0.3738×10^{-1}	0.170	0.823045×10^{1}	0.1063×10^{3}
L(0,t)	0.200×10^{2}	0.200004×10^{2}	0.1354×10^{-1}	0.180×10^{2}	0.228788×10^{2}	0.5643×10^{2}

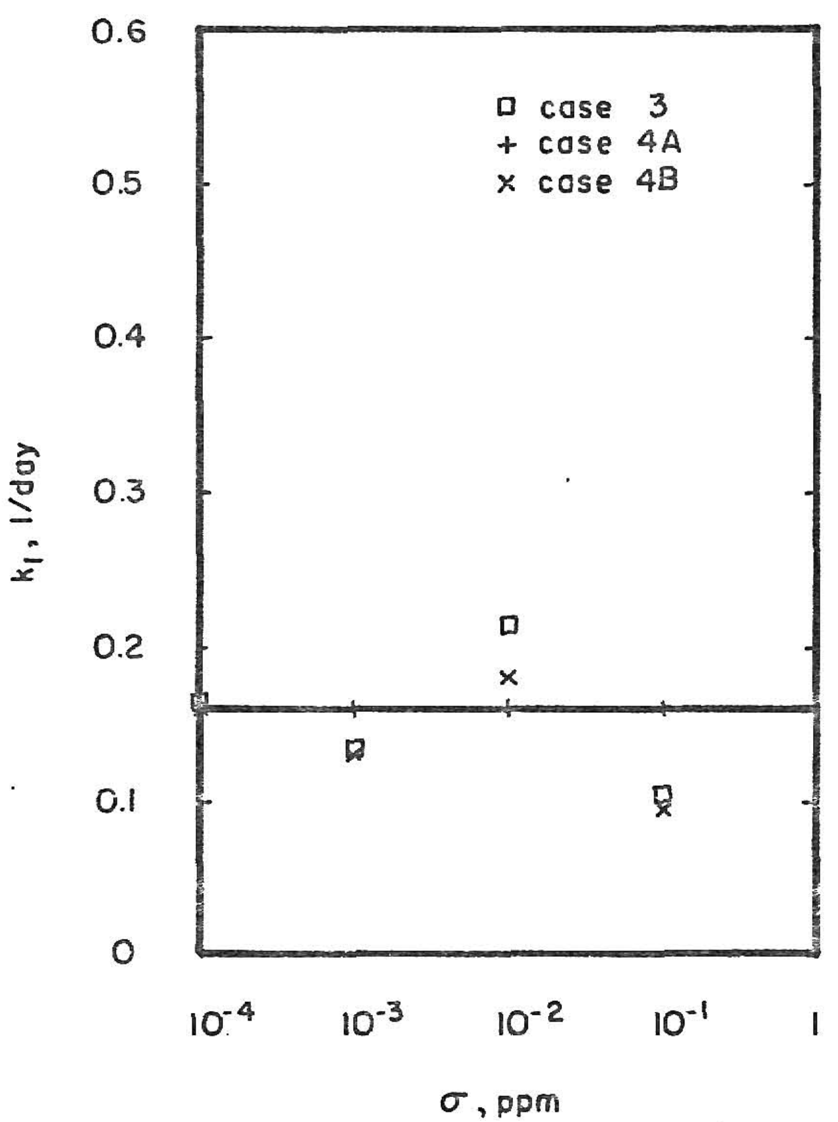


Fig. 3.7 Estimated values of k_1 as a function of σ for Cases 3 and 4

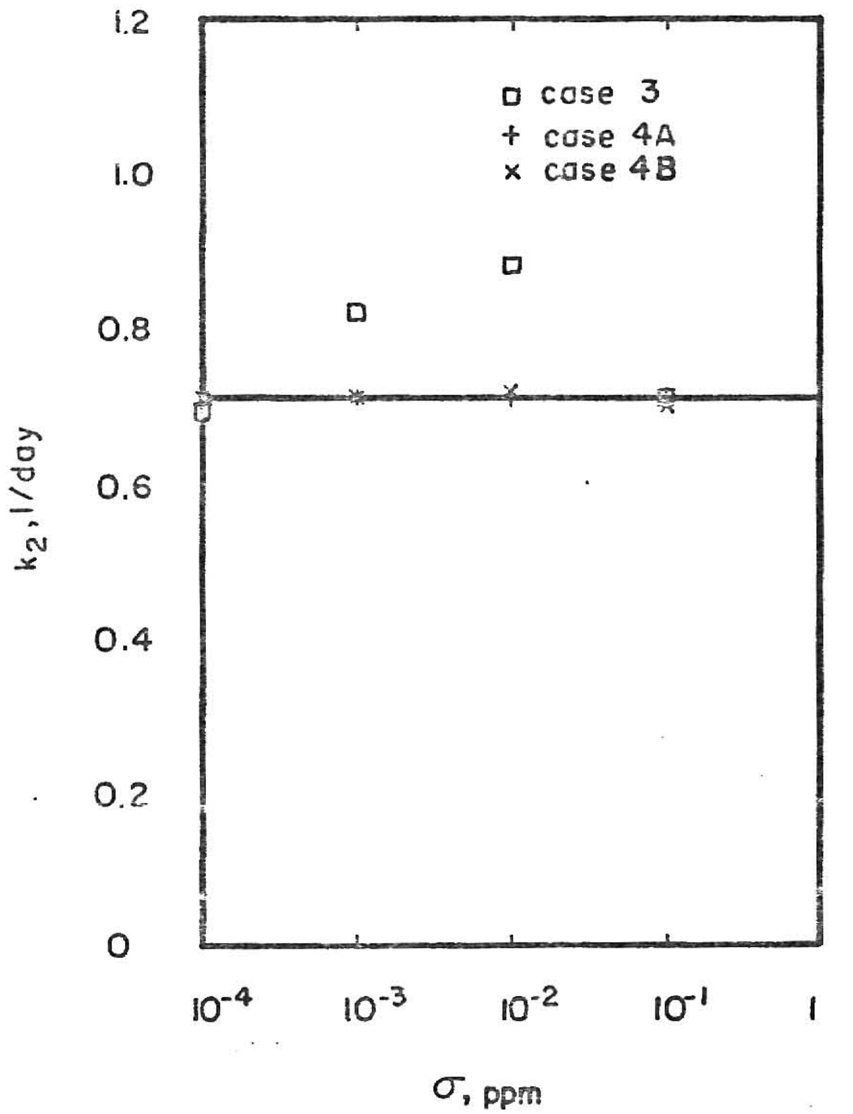


Fig. 3.8 Estimated values of k_2 as a function of σ for Cases 3 and 4

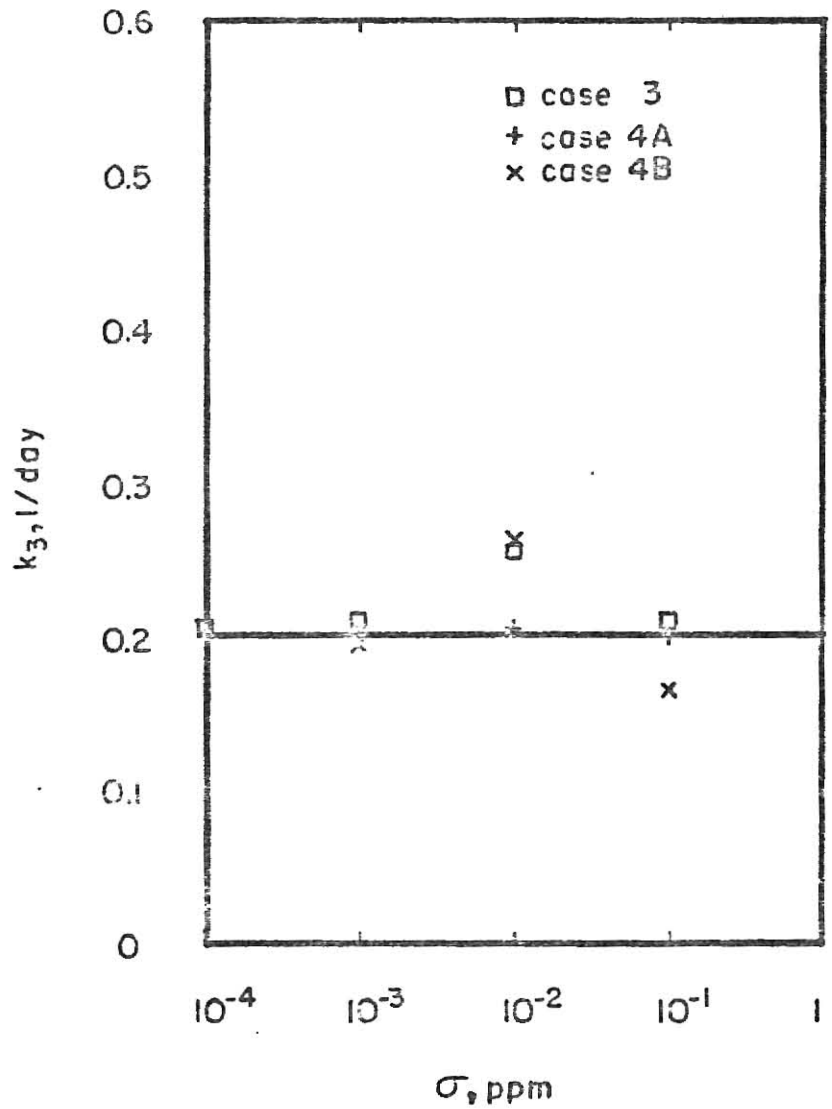


Fig.3.9 Estimated values of k_3 as a function of σ for Cases 3 and 4

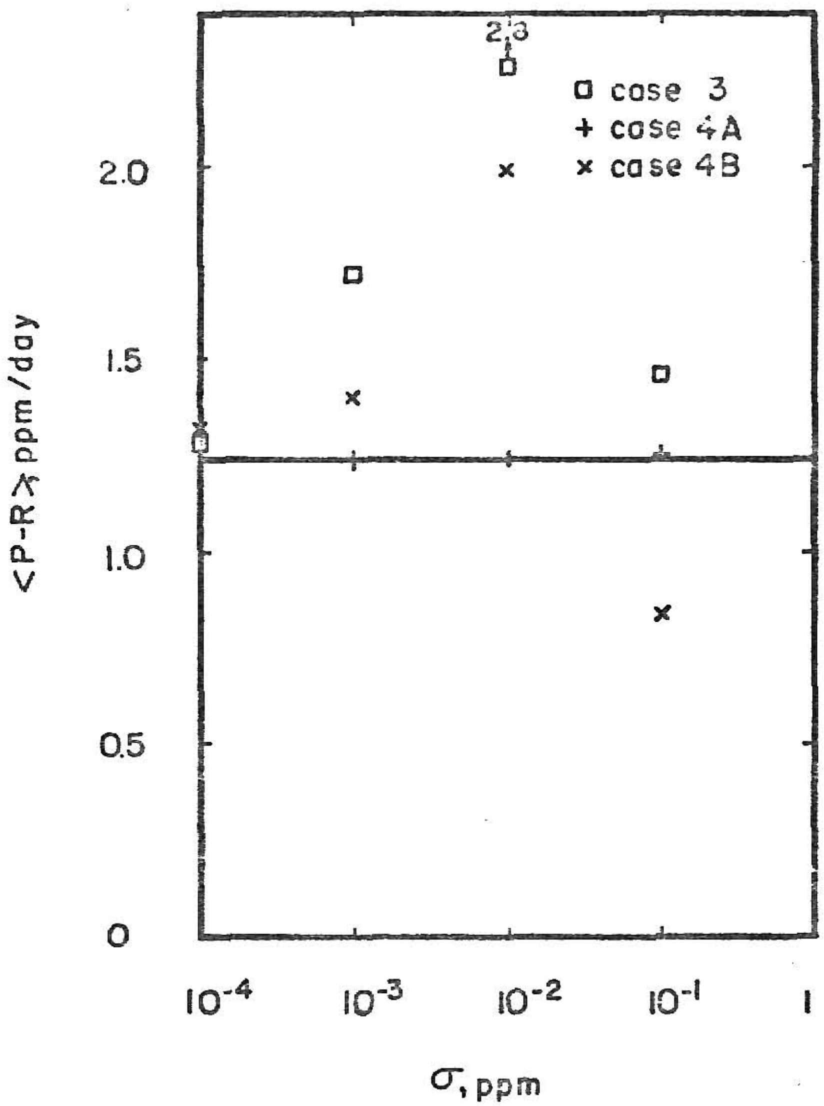


Fig. 3.10 Estimated values of <P-R> as a function of σ for Cases 3 and 4

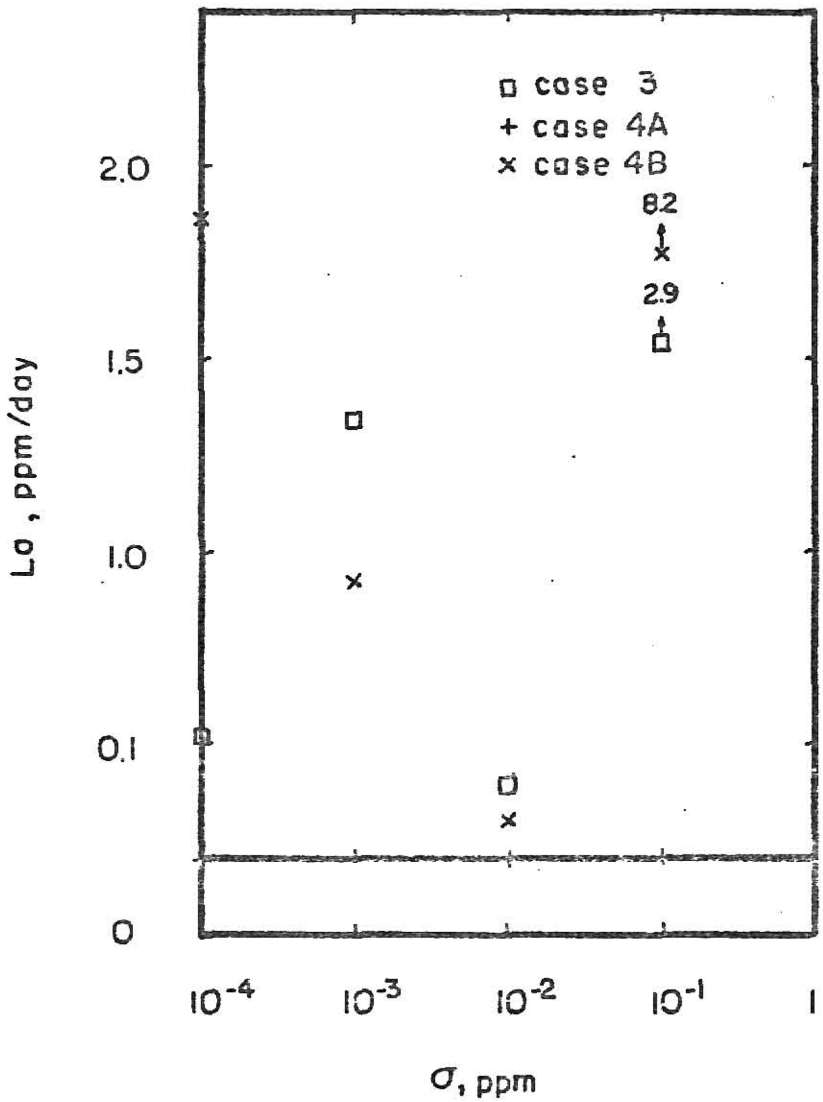


Fig. 3.11 Estimated values of La as a function of σ for Cases 3 and 4

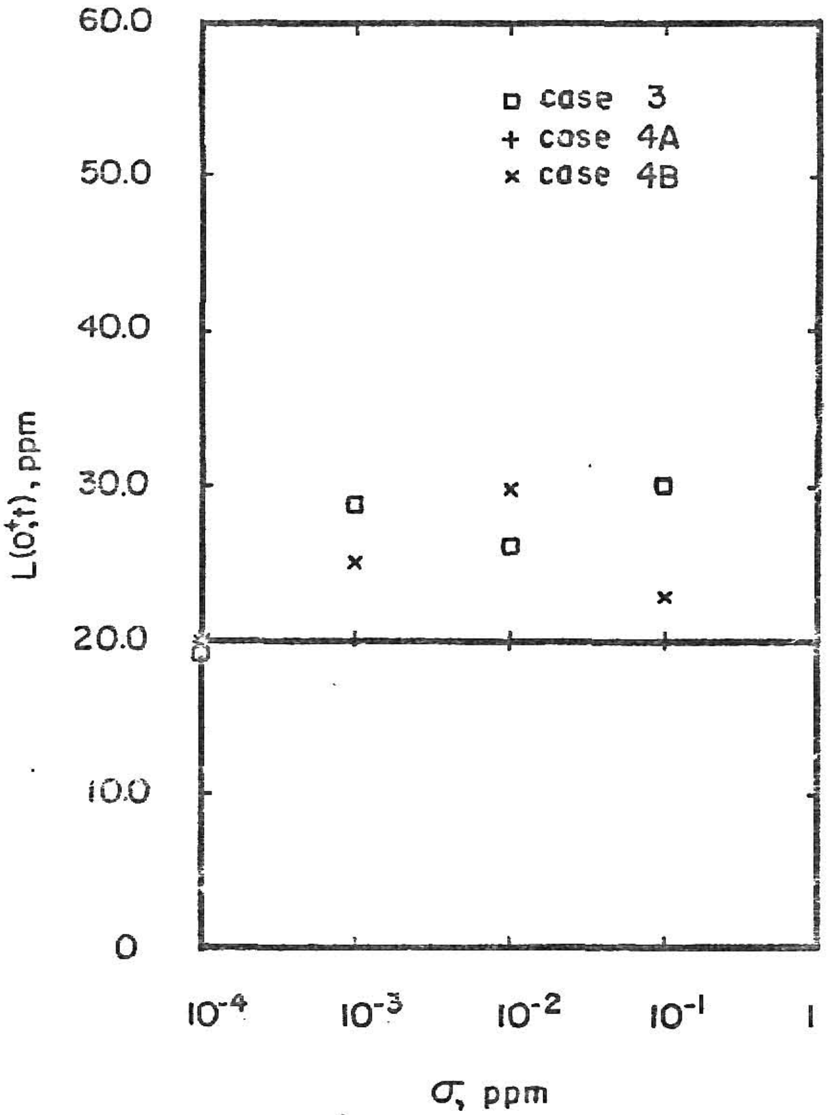


Fig.3.12 Estimated values of $L(0^+,t)$ as a function of σ for Cases 3 and 4

the parameter estimates for Case 4B. The actual value of the parameters are represented by the solid line. The minimized criterion function [see equation (3.14)] as a function of σ is shown in Fig. 3.13, for Cases 3, 4A, and 4B.

3.6 ANALYSIS AND DISCUSSION

An examination of the results presented in Tables 3.4 through 3.15 and illustrated in Figs. 3.4 through 3.13 reveals that, in general, the estimated values of the parameters differ from the actual or nominal values for all the cases except for Cases 2 and 4A for which deviations are negligible. It is convenient to initiate the discussion of these results by examining firstly some properties of BOD and DO data in the time domain before examining the deviations observed for the parameter estimates. These deviations will be discussed under the headings: effect of type of input on parameter estimation and effect of number of parameters.

Properties of BOD and DO Data in the Time Domain: In general, two quantities are correlated when they exhibit behavior patterns at the same time, or with some time lag between them. BOD and DO, when measured at two monitoring stations x_1 miles apart, are good examples of events that are correlated at different times (Shastry et al., 1972). If a suitable time lag or time difference $\tau = x_1/u$ is used, the observations from the two stations will correlate well; but for other time lags the correlation will be poor. These properties have been used in this study to correlate BOD data (Cases 1 and 2) and DO data (Cases 3 and 4) measured at two locations, $x = 0^+$ and $x = x_1$.

Effect of Type of Input on Parameter Estimation: One of the most elementary ways of testing correlation is the use of a scatter diagram.

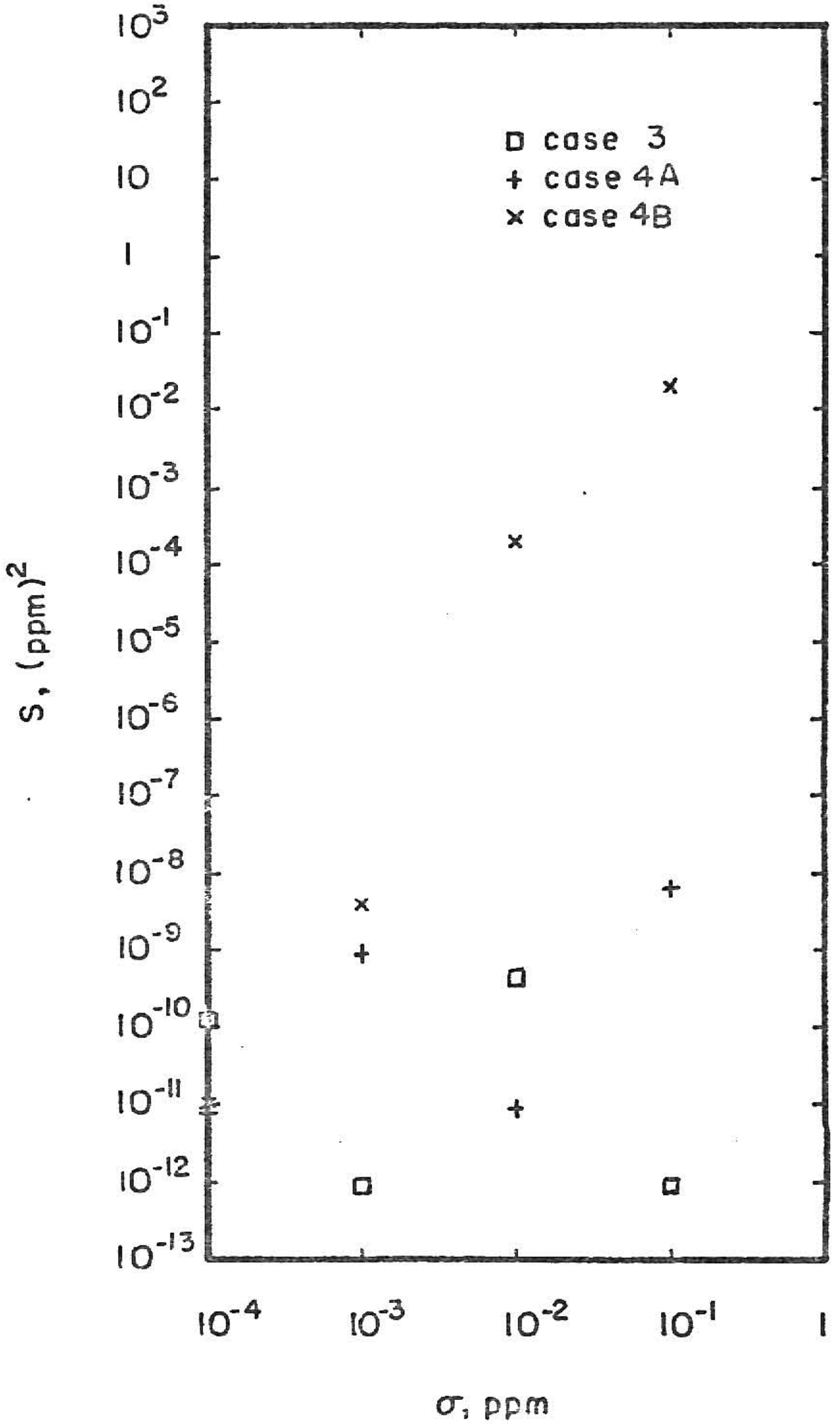


Fig.3.13 Estimated values of S as a function of σ for Cases 3 and 4

Paired observations of the water quality variable considered for a given case (BOD for Cases 1 and 2, and DO for Cases 3 and 4), measured at $x = 0^+$ (input variable) and $x = x_1$ (output variable), can be used to construct the diagram. In this diagram, the output variable is plotted as a function of the input variable as in Fig. 3.2, for example. If the points tend to fall on a single line, the two variables are correlated. If they are distributed truly randomly there is no correlation. This test was applied in all the cases considered. It was observed for all cases that the points fell essentially on a single line. However, the length of such a line obtained from Cases 1 or 3 was smaller than the length from the other two cases. These results are attributed to the type of input function used to represent the deterministic signal of BOD (Cases 1 and 2) and DO (Cases 3 and 4). The length of the line is also a function of the standard deviation of the stochastic input signal.

A constant parameter linear system was used in this study. It is worth noting that the correlation analysis for this system was carried out in the time domain and the results of this analysis were found to be dependent on both the time lag τ, and the type of input used to excite the system. If the analysis had been carried out in the frequency domain, the results would depend only on the frequency and will not be affected by either time or the type of input used to excite the system. This phenomenon is characteristic of constant parameter linear systems (Bendat and Piersol, 1971). However, for non-linear systems or systems described by time-varying parameters, the frequency response will be a function of both the applied input signal and time. A further discussion on frequency response is avoided since the correlation analysis was carried out in the time domain.

The application of the procedure presented in Section 3.4 to estimate the parameters in equations (3.10) and (3.11) has its limitations. A reasonable spread of the data in the scatter diagram is needed for parameter estimation. It is obvious that a step input does not give the necessary spread in the data needed for parameter estimation whereas a cyclic input does. This spread in the data can also be achieved by using a generalized input. It is apparent that the standard deviation of the stochastic signal contributes to the deviation of the parameter estimates. However, the biggest contribution comes from the type of deterministic input signal used. This can be observed for example, in Table 3.16 where deviations for Cases 1 and 2 are compared. The same reasoning can be applied to Cases 3, 4A and 4B. However, Cases 4A and 4B (see Table 3.17) show noticeable deviations of parameter estimates despite the fact that simulation conditions were similar to the conditions used for Case 2. These results are discussed in the next paragraph.

Effect of Number of Parameters in the Estimation Procedure: In Cases 3, 4A and 4B six parameters were estimated from DO data using the procedure presented in Section 3.4. When more than two parameters are being estimated simultaneously the computation becomes more involved. The search has to be done in six-dimensions since six parameters are being estimated. In this case it is difficult to predict whether the true minimum of the criterion function S can be obtained, which gives a measure of the goodness of the parameter estimates. The deviations observed for Case 3 (see Table 3.17) are due in part to the difficulty found in the search but the most important contribution to these deviations comes from the type of input used. The results obtained for Case 4A are similar to the results obtained from Case 2 (see Tables 3.16 and 3.17) in that the deviation of the parameter estimates

Table 3.16 Deviation Percentages of the Parameters from their Actual Values

Case 1 and 2*

Parameter	Case 1				Case 2			
	Standard Deviation, σ				Standard Deviation, σ			
	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
k_r	-11	+ 5	-12	-22	-10^{-3}	-10^{-3}	-10^{-3}	-5×10^{-3}
τ	+13	- 5	+15	+30	$+10^{-4}$	-10^{-4}	$+10^{-4}$	$+10^{-4}$

*In these calculations, a positive sign means that the parameter was overestimated and a negative sign means that the parameter was underestimated.

Table 3.17 Deviation Percentages of Parameters from their Actual Values

Cases 3, 4A and 4B*

Parameter	Case 3				Case 4A				Case 4B			
	Standard Deviation, σ				Standard Deviation, σ				Standard Deviation, σ			
	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
k_1	+ 5	-15	+37	-34	-10^{-3}	$+10^{-3}$	$+10^{-2}$	$+10^{-2}$	+0.3	-18	+14	-41
k_2	- 3	+15	+23	$+10^{-3}$	$+10^{-3}$	0	$+10^{-3}$	0	$+10^{-3}$	$+10^{-3}$	+0.6	- 2
k_3	+ 5	+ 4	+27	+ 4	$+10^{-3}$	$+10^{-3}$	$+10^{-3}$	$+10^{-3}$	+ 5	- 3	+32	-18
<P-R>	+ 3	+38	+100	+17	-10^{-3}	$+10^{-2}$	+0.2	$+10^{-2}$	+ 5	+12	+59	-32
La	+160	+580	+95	+44	+ 2	$+10^{-3}$	+0.7	+0.2	- 7	+359	+48	+400
L(0,t)	- 5	+44	+30	+95	-10^{-3}	-10^{-3}	$+10^{-2}$	$+10^{-3}$	- 2	+25	+18	+14

*In these calculations, a positive sign means that the parameter was overestimated and a negative sign means that the parameter was underestimated.

are negligible. This is mainly due to the fact that in Case 4A the nominal values of the parameters were used as the initial guesses for the iterative procedure. The use of these initial guesses reduced greatly the difficulties of a six-dimensional search. The results from Case 4B can be atributed to the computational difficulties found in the search.

3.7 CONCLUDING REMARKS

A new approach to estimate parameters appearing in time-varying or transient water quality models has been presented. Estimates were obtained by using Bard's method for parameter estimation. It is apparent that the parameter estimates deviate from their nominal values depending upon the characteristics of the input signal used to excite the system and the number of parameters being estimated simultaneously. It will be of interest to investigate the use of noise corrupted measurements for parameter estimation using the approach presented in this study. In addition, the use of other methods for computing the parameter estimates should be investigated and the results compared with estimates obtained with Bard's method.

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APPENDIX 3.1

THE METHOD OF CHARACTERISTICS

In this Appendix, a brief description of the method of characteristics is presented. It is based on the description given by Abbot (1966). Consider the following convective transport equation

$$\frac{\partial z}{\partial t} + B(x,t)\,\frac{\partial z}{\partial x} = C(x,t,z) \tag{A-3.1.1}$$

Let the region of integration of (A-3.1.1) be a space with three dimensions, with coordinates t, x, z. If z is treated as the dependent variable, with t and x independent, we have two "principal slopes," namely $\partial z/\partial t$ in the t direction and $\partial z/\partial x$ in the x direction. These slopes together define the increment dz in terms of the increments dt and dx, by

$$dz = \frac{\partial z}{\partial t}dt + \frac{\partial z}{\partial x}dx \tag{A-3.1.2}$$

which, when p is written for $\partial z/\partial t$ and q for $\partial z/\partial x$ becomes

$$dz = pdt + qdx \tag{A-3.1.3}$$

The slopes p and q define the orientation of a planar surface in the t-x-z space. For each point P(t,x,z) in the t-x-z space, the partial differential equation does not define unique values of p and q. Equation (A-3.1.1) merely expresses a relation between p and q. This equation may be written as

$$Ap + Bq + C \tag{A-3.1.4}$$

where B and C may be functions of t, x, and z, and A = 1. The planar elements may be obtained by substituting related pairs of values p and q in (A-3.1.3). Thus, treating (A-3.1.2) and (A-3.1.4) as a pair of simultaneous equations for p and q, a set of planar elements may be defined. From Fig. (A-3.1) it can be seen that these planar elements will intersect along a line such as EF. The slopes p and q may then have any values depending upon the selection of the planes. Thus, the unique values of p and q do not exist, they are undeterminated, although (A-3.1.2) and (A-3.1.4) hold along this line.

Equations (A-3.1.2) and (A-3.1.4) become

$$\begin{bmatrix} A & B \\ dt & dx \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} C \\ dz \end{bmatrix} \qquad \text{(A-3.1.5)}$$

If they are linearly dependent the following relations must be satisfied:

$$\begin{vmatrix} A & B \\ dt & dx \end{vmatrix} = 0$$

$$\begin{vmatrix} A & C \\ dt & dz \end{vmatrix} = 0$$

and

$$\begin{vmatrix} C & B \\ dz & dx \end{vmatrix} = 0$$

i.e.

$$\frac{dt}{A} = \frac{dx}{B} = \frac{dx}{C} \qquad \text{(A-3.1.6)}$$

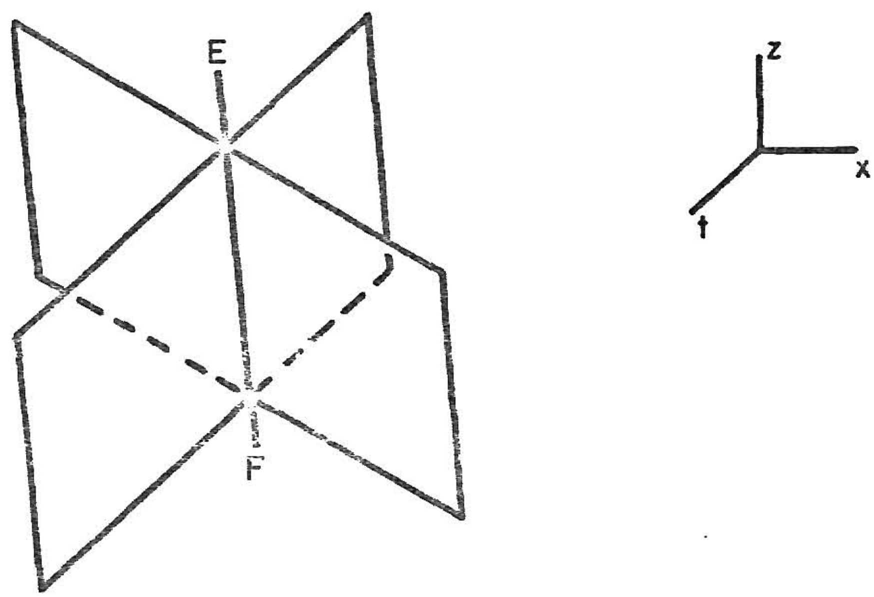


Fig. A-3.1 The characteristic ruling as a line of interception of two planar elements.

Equation (A-3.1.6) represents the line which is common to all planar elements. This is called the characteristic line or the characteristic of zero order. The slope of the "Base characteristic," dx/dt, is given by

$$\frac{dx}{dt} = \frac{B}{A} = B \tag{A-3.1.7}$$

Equation (A-3.1.7) is the base line along which (A-3.1.1) is integrated.

This can be interpreted physically as follows: Consider a small drop of water flowing downstream. The relation of the position and the elapsed time of the water drop is described by (A-3.1.7), but the change in concentration (assuming z represents concentration of the drop) inside the water drop by physical and chemical processes is represented by

$$\frac{dz}{dt} = C(x) \tag{A-3.1.8}$$

This concludes the description of the method of characteristics.

APPENDIX 3.2

ANALYTICAL SOLUTION OF THE SYSTEMS EQUATIONS

By applying the method of characteristics to the system equations (3.1) and (3.2) the set of partial differential equations is transformed into a set of ordinary differential equations.

$$\frac{dx}{dt} = u \tag{A-3.2.1}$$

$$\frac{dL}{dt} = -(k_1 + k_3)\ L + La \tag{A-3.2.2}$$

$$\frac{dC}{dt} = -k_1 L + k_2\ (C_s - C) + \langle P\text{-}R \rangle \tag{A-3.2.3}$$

where equation (A-3.2.1) is the characteristic line along which equations (A-3.2.2) and (A-3.2.3) are integrated. These two equations can be written in vector form as

$$\frac{d}{dt}\ z(x,t) = k\ z(x,t) + S(x,t) \tag{A-3.2.4}$$

with

$$z(x,t) = \begin{bmatrix} L(x,t) \\ \\ C(x,t) \end{bmatrix} \tag{A-3.2.5}$$

$$K = \begin{bmatrix} -(k_1 + k_3) & 0 \\ \\ -k_1 & -k_2 \end{bmatrix} \tag{A-3.2.6}$$

and

$$S(x,t) = \begin{bmatrix} La \\ \\ k_2 C_s + \langle P\text{-}R \rangle \end{bmatrix} \tag{A-3.2.7}$$

Assuming that the system is time invariant, i.e., its characteristic line does not change with time, the solution of equation (A-3.2.4) may be expressed by (Zadeh and Desoer, 1963)

$$z(x,t) = \psi(t, t_o)\, z(x_o, t_o) + \int_{t_o}^{t} \psi(t,\sigma)\, S[x(\sigma), \sigma]\, d\sigma \tag{A-3.2.8}$$

where the matrix $\psi\,(t, t_o)$ is defined by

$$\frac{d\psi(t,t_o)}{dt} = K\,\psi(t,t_o) \tag{A-3.2.9}$$

$$\psi(t_o, t_o) = I \quad \text{(Identity matrix)}$$

This same procedure was followed by Koivo and Phillips (1971) without considering some source and sinks such as local runoff and sedimentation. The solution of equation (A-3.2.9) yields:

$$\psi(t, t_o) = \begin{bmatrix} e^{-(k_1 + k_3)\,(t - t_o)} & 0 \\ \dfrac{-k_1[e^{-(k_1+k_3)(t-t_o)} - e^{-k_2(t-t_o)}]}{k_2 - (k_1 + k_3)} & e^{-k_2(t-t_o)} \end{bmatrix} \tag{A-3.2.10}$$

Performing the integration of the second term of the right hand side of equation (A-3.2.8) it is obtained

$$\int_{t_o}^{t} \psi S d\sigma = \int_{t_o}^{t} \begin{bmatrix} e^{-(k_1+k_3)(t-\sigma)} & 0 \\ -\dfrac{k_1\left\{e^{-(k_1+k_3)(t-\sigma)} - e^{-k_2(t-\sigma)}\right\}}{k_2 - (k_1+k_3)} & e^{-k_2(t-\sigma)} \end{bmatrix} \begin{bmatrix} La \\ k_2 C_s + \langle P-R \rangle \end{bmatrix} d\sigma$$

$$= \begin{bmatrix} \dfrac{La}{k_1+k_3}\left\{1-e^{-(k_1+k_3)(t-t_o)}\right\} \\ \dfrac{-k_1 La}{k_2-(k_1+k_3)}\left\{\dfrac{(1-e^{-(k_1+k_3)(t-t_o)})}{k_1+k_3} - \dfrac{(1-e^{-k_2(t-t_o)})}{k_2}\right\} + \left\{C_s + \dfrac{\langle P-R \rangle}{k_2}\right\}\left\{1-e^{-k_2(t-t_o)}\right\} \end{bmatrix} \quad \text{(A-3.2.11)}$$

The complete expression may be written as

$$\begin{bmatrix} L(x,t) \\ C(x,t) \end{bmatrix} = \begin{bmatrix} e^{-(k_1+k_3)(t-t_o)} & 0 \\ \dfrac{k_1\left\{e^{-(k_1+k_3)(t-t_o)} - e^{-k_2(t-t_o)}\right\}}{k_2-(k_1+k_3)} & e^{-k_2(t-t_o)} \end{bmatrix} \begin{bmatrix} L(x_o,t_o) \\ C(x_o,t_o) \end{bmatrix}$$

$$+ \begin{bmatrix} \dfrac{La}{k_1+k_3}\left\{1-e^{-(k_1+k_3)(t-t_o)}\right\} \\ \dfrac{-k_1 La}{k_2-(k_1+k_3)} \left\{\dfrac{(1-e^{-(k_1+k_3)(t-t_o)})}{k_1+k_3} - \dfrac{(1-e^{-k_2(t-t_o)})}{k_2}\right\} + \left\{C_s + \dfrac{\langle P-R\rangle}{k_2}\right\}\left\{1-e^{-k_2(t-t_o)}\right\} \end{bmatrix} \qquad \text{(A-3.2.12)}$$

or, after rearranging

$$L(x,t) = L(x_o,t_o)e^{-(k_1+k_3)(t-t_o)} + \frac{La}{k_1+k_3}\left[1-e^{-(k_1+k_3)(t-t_o)}\right] \qquad \text{(A-3.2.13)}$$

$$C(x,t) = C_s(1-e^{-k_2(t-t_o)}) - \frac{k_1[L(x_o,t_o) - \frac{La}{k_1+k_3}]}{k_2-(k_1+k_3)}[e^{-(k_1+k_3)(t-t_o)} - e^{-k_2(t-t_o)}]$$

$$+\frac{1}{k_2}[<P-R> - \frac{k_1La}{k_1+k_3}][1-e^{-k_2(t-t_o)}] + C(x_o,t_o)e^{-k_2(t-t_o)} \quad \text{(A-3.2.14)}$$

Application of the boundary conditions to equations (A-3.2.13) and (A-3.2.14) yields (a) for $0 \le t \le x/u$ (initial condition along the $t=0$ axis), with $t_o = 0$,from (A-3.2.1), $x_o = x-ut$.

then

$$L(x,t) = L(x-ut,0)e^{-(k_1+k_3)t} + \frac{La}{k_1+k_3}[1-e^{-(k_1+k_3)t}] \quad \text{(A-3.3.15)}$$

$$C(x,t) = C_s(1-e^{-k_2t}) - \frac{k_1[L(x-ut,0) - \frac{La}{k_1+k_3}]}{k_2-(k_1+k_3)}[e^{-(k_1+k_3)t} - e^{-k_2t}]$$

$$+\frac{1}{k_2}[<P-R> - \frac{k_1La}{k_1+k_3}][1-e^{-k_2t}] + C(x,ut,o)\,e^{-k_2t} \quad \text{(A-3.2.16)}$$

(b) for $t \geq x/u$ (initial condition along the $x = 0$, axis), with $x_o = 0$

from A-3.2.2.1), $t_o = t - x/u$

then

$$L(x,t) = L(0,t-x/u)e^{-(k_1+k_3)\,x/u} + \frac{La}{k_1+k_3}[1-e^{-(k_1+k_3)x/u}] \quad \text{(A-3.2.17)}$$

$$C(x,t) = C_s(1-e^{-k_2 x/u}) - \frac{k_1[L(0,t-x/u) - \frac{La}{k_1+k_3}]}{k_2-(k_1+k_3)} [e^{-(k_1+k_3)x/u} - e^{-k_2 x/u}]$$

$$+ \frac{1}{k_2} [<P-R> - \frac{k_1 La}{k_1+k_3}] [1-e^{-k_2 x/u}] + C(0,t-x/u)\, e^{-k_2 x/u} \qquad \text{(A-3.2.18)}$$

It is worth noting that no constraints have been applied to the initial BOD and DO conditions (at $x=0^+$) in equations (A-3.3.17) and (A-3.2.18). They can be any arbitrary function of time. This concludes Appendix 3.2.

APPENDIX 3.3

STREAM AFFECTED BY MULTIPLE DISCHARGES

A system affected by multiple discharges may be treated as an extension of the system treated in Section 3.2. The following description is based on the one given by Fan et al. (1971) using the dispersion model.

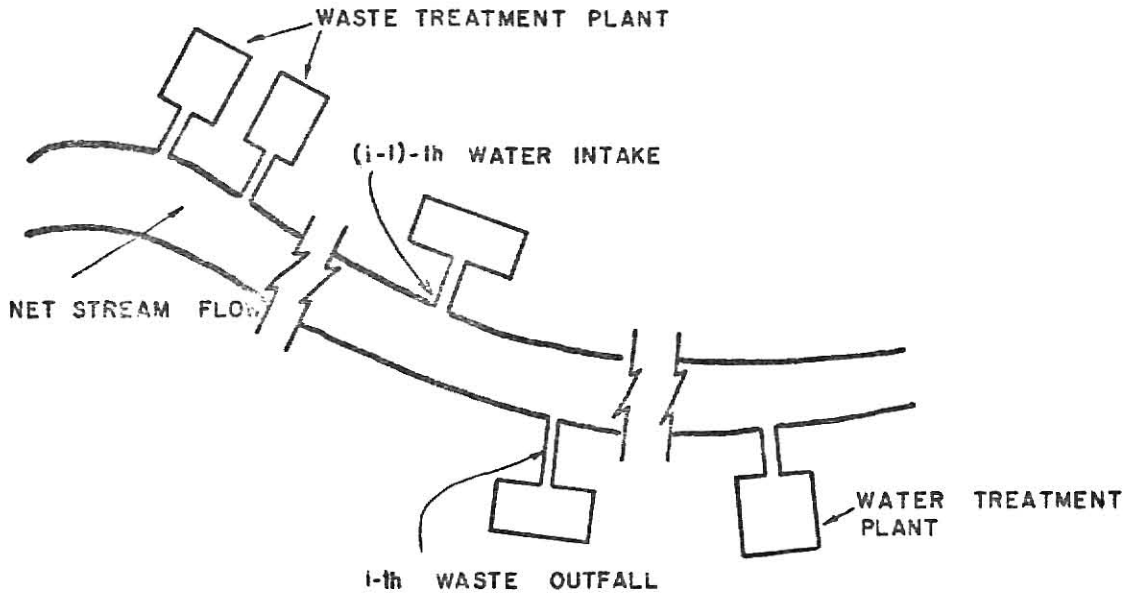
Consider a stream with several waste outfalls and water intakes, as shown in Fig. (A-3.3.1). For the purpose of analysis the stream is divided into (n + m + 1) sections, where n is the number of waste outfalls and m the number of water intakes. Every section begins just below a new outfall or intake. Equations (3.1) and (3.2), of Chapter 3, applied to the i-th section can be written as

$$\frac{\partial L^i}{\partial t} + u^i \frac{\partial L^i}{\partial x} + (k_1{}^i + k_3{}^i)\, L^i - L_a{}^i = 0 \qquad \text{(A-3.3.1)}$$

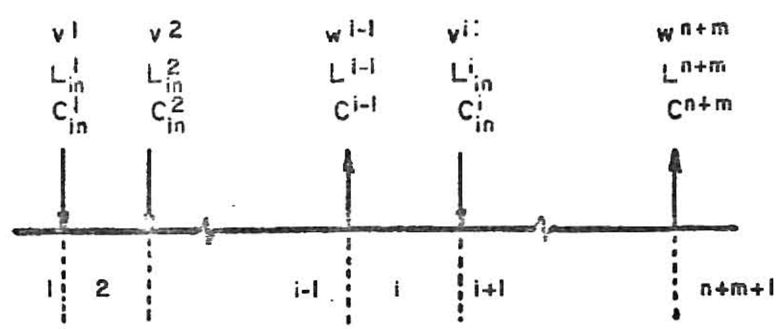
$$\frac{\partial C^i}{\partial t} + u^i \frac{\partial C^i}{\partial x} + k_1{}^i L^i - k_2{}^i\,(C_s{}^i - C^i) - (P - R)^i = 0 \qquad \text{(A-3.3.2)}$$

where the superscript i denotes properties in the i-th section, and u is the mean velocity of the stream. Parameters may change from section to section because of changes in flow pattern, bacterial activity, etc. The advantage gained by using this scheme is similar to that gained in difference modeling.

For regions near the waste outfalls, the input can be visualized as a side stream injected into an open flow system. The mixing at the



(a) Stream with several waste outfalls and water intakes



(b) One-dimensional representation of the above system

Fig. A-3.3.1 Representation of a stream with several waste inputs and water intakes point of entry is assumed to be instantaneous and complete in keeping with the other assumptions of the model. The boundary conditions are (Yano et al., 1968).

For a waste input at $x = x_i$ between the i-th and (i + 1)-th sections,

$$(L^i)_{x \to x_i^-} = (L^{i+1})_{x \to x_i^+} \tag{A-3.3.3}$$

$$(C^i)_{x \to x_i^-} = (C^{i+1})_{x \to x_i^+} \tag{A-3.3.4}$$

Equations (A-3.3.3) and (A-3.3.4) represent the continuity of concentration profile. Because of the continuity of flux of material across $x = x_i$,

$$(u^i L^i A^i)_{x \to x_i^-} + (v^i L^i_{in} A^i)_{x = x_i} = (u^{i+1} L^{i+1} A^{i+1})_{x \to x_i^+} \tag{A-3.3.5}$$

$$(u^i C^i A^i)_{x \to x_i^-} + (v^i C^i_{in} A^i)_{x = x_i} = (u^{i+1} C^{i+1} A^{i+1})_{x \to x_i^+} \tag{A-3.3.6}$$

where v^i is the volumetric flow rate of the waste per unit are of the stream, L_{in} and C_{in} are its BOD and DO concentrations, respectively. It may be noted that the reaction terms are absent since the material balance is over a section which has essentially zero volume.

Similarly, for water intake at $x = x_j$ between the j-th and the (j+1)-th sections,

$$(L^j)_{x \to x_j^-} = (L^{j+1})_{x \to x_j^+} \qquad \text{(A-3.3.7)}$$

$$(C^j)_{x \to x_j^-} = (C^{j+1})_{x \to x_j^+} \qquad \text{(A-3.3.8)}$$

$$(u^j L^j A^j)_{x \to x_j^-} - (w^j L^j A^j)_{x = x_j} = (u^{j+1} L^{j+1} A^{j+1})_{x \to x_j^+} \qquad \text{(A-3.3.9)}$$

$$(u^j C^j A^j)_{x \to x_j^-} - (w^j C^j A^j)_{x = x_j} = (u^{j+1} C^{j+1} A^{j+1})_{x \to x_j^+} \qquad \text{(A-3.3.10)}$$

where w^j is the volumetric flow rate of water intake per unit area of the stream.

To solve for the BOD and DO profiles for the $(n + m + 1)$ sections, the PDEs [given by equations (A-3.3.1) and (A-3.3.2)] for every section must be solved. Applying the method of characteristics the solutions to equations (A-3.3.1) and (A-3.3.2) are given by

$$L(x_i, t) = L(x_i - u^i t, 0) \exp \{-(k_1^i + k_3^i)t\}$$

$$+ \frac{L_a^i}{k_1^i + k_3^i} [1 - \exp \{-(k_1^i + k_3^i)t\}] \qquad \text{(A-3.3.11)}$$

$$C(x_i, t) = C_s^i [1 - \exp \{-k_2^i t\}] - \frac{k_1^i \left[L(x_i - u^i t, 0) - \dfrac{L_a}{k_1^i + k_3^i} \right]}{k_2^i - (k_1^i + k_3^i)}$$

$$[\exp \{-k_1^i + k_3^i)t\} - \exp \{-k_2^i t\}] + \frac{1}{k_2^i} \left[(P - R)^i - \frac{k_1^i L_a^i}{k_1^i + k_3^i} \right]$$

$$[1 - \exp \{-k_2^i t\}] + C\,(x_i - u^i t;\ 0) \exp \{-k_2^i t\} \qquad \text{(A-3.3.12)}$$

(b) For $t \geq x_i/u^i$ (Initial condition along the x = 0 axis)

$$L(x_i, t) = L(0, t - \frac{x_i}{u^i}) \exp\left\{-(k_1^{\,i} + k_3^{\,i})\frac{x_i}{u^i}\right\}$$

$$+ \frac{L_a^{\,i}}{k_1^{\,i} + k_3^{\,i}}\left[1 - \exp\left\{-(k_1^{\,i} + k_3^{\,i})\frac{x_i}{u^i}\right\}\right] \qquad \text{(A-3.3.13)}$$

$$C(x_i, t) = C_s^{\,i}\left[1 - \exp\left\{-k_2^{\,i}\frac{x_i}{u^i}\right\}\right] - \frac{k_1^{\,i}\left[L(0, t - \frac{x_i}{u^i}) - \frac{L_a^{\,i}}{k_1^{\,i} + k_3^{\,i}}\right]}{k_2^{\,i} - (k_1^{\,i} + k_3^{\,i})}$$

$$\left[\exp\left\{-(k_1^{\,i} + k_3^{\,i})\frac{x_i}{u^i}\right\} - \exp\left\{-k_2^{\,i}\frac{x_i}{u^i}\right\}\right]$$

$$+ \frac{1}{k_2^{\,i}}\left[\langle P-R\rangle^i - \frac{k_1^{\,i}L_a^{\,i}}{k_1^{\,i} + k_3^{\,i}}\right]\left[1 - \exp\left\{-k_2^{\,i}\frac{x_i}{u^i}\right\}\right] + C(0, t - \frac{x_i}{u^i})$$

$$\exp\left\{-k_2^{\,i}\frac{x_i}{u^i}\right\} \qquad \text{(A-3.3.14)}$$

This concludes Appendix 3.3.

APPENDIX 3.4

THE GAUSS-NEWTON METHOD (BARD'S METHOD)

The Gauss-Newton method, with modification by Greenstadt-Eisenpress (1963), Bard (1967), and Carroll (1961) is used for minimizing the selected criterion function. This can be also accomplished by maximizing a function $G(\theta) = - S(\theta)$. This method is generally known as Bard's Method (1967). A brief description is given below.

The maximization of the $G(\theta)$ proceeds in an iterative fashion. At each iteration we start with an initial guess $\theta^{(1)}$ such that $G(\theta^{(1)}) > G(\theta^{(0)})$. This now becomes the initial guess for the next iteration. In the course of iteration two things must be determined: a direction $\Delta\theta$ to proceed in, and length λ of the step to be taken along this direction, so that $\theta^{(1)} = (\theta^{(0)} + \lambda\ \Delta\theta)$. To be acceptable, the direction must be such that as one proceeds along it from $\theta^{(0)}$ the value of G - function increases at least initially, i.e., for sufficiently small λ. The value of λ is ideally such that as to take us near the peak of G along the chosen direction. The other requirement being that, λ must be small enough to insure that $\theta^{(1)}$ satisfies all bounds and constraints on θ.

Choice of Direction

Let P be the vector of partial derivatives $\frac{\partial G}{\partial \theta}$ at $\theta = \theta^{(0)}$. If R is any positive definite matrix, the direction $\Delta\theta = R_P$ is easily shown to be acceptable. If $\theta^{(0)}$ is sufficiently near a maximum of G, the matrix $Q_{ij} = -\frac{\partial^2 G}{\partial \theta_i \partial \theta_j}$ is positive (or at least non-negative) definite, and it can be shown that Q^{-1} is the most efficient choice of R. Using $R = Q^{-1}$ at all points constitutes the Newton-Raphson method. In regions where Q is not positive definite this method is likely to yield non-acceptable directions, and hence fail to converge.

This problem can be overcome according to Greenstadt (1963) if one represents the matrix Q by means of its eigenvalues and eigenvectors:

$$Q_{ij} = \sum_k V_{ik} V_{jk} \mu_k \tag{A-3.4.1}$$

where

$V_{ik} = i^{th}$ element of the k^{th} eigenvector of Q

$V_{jk} = j^{th}$ element of the k^{th} eigenvector of Q

$\mu_k = k^{th}$ eigenvalue of Q

Now setting:

$$R_{ij} = \sum_k V_{ik} V_{jk} |\mu_k|^{-1} \tag{A-3.4.2}$$

This R is always positive definite, and coincides with Q where the latter is itself positive definite, i.e., around the maximum. It is important to note that if some μ_k is zero, this value is replaced by a small, non-zero number.

Choice of Step Size

As Stated above, we computed $\Delta\theta = R_p$, with R as defined by Equation (A-3.4.2). Let λ_o be a positive number such that $(\theta^{(0)} + \lambda_o \Delta\theta)$ is in the acceptable region. Now set $\lambda_2 = \min(\lambda_o, 1)$ and $\theta^{(2)} = (\theta^{(0)} + \lambda_2\Delta\theta)$. Define $\Gamma(\lambda) = G[\theta^{(0)} + \lambda\,\Delta\theta]$. Then $(0) = G(\theta^{(0)})$; $\Gamma(\lambda_2) = G(\theta^{(2)})$; and

$$\frac{d\Gamma}{d\lambda}\Big|_{\lambda=0} = \frac{\partial G}{\partial\theta}\Big|_{\theta=\theta^{(0)}} \cdot \Delta\theta = p \cdot \Delta\theta = \sum_i p_i \Delta\theta_i$$

$\Gamma(\lambda)$ can be approximated by a parabola $(a + b\lambda + c\lambda^2)$ matching the values of the parabola at $\lambda = 0$ and $\lambda = \lambda_2$, and its derivatives at $\lambda = 0$ with corresponding known quantities of the function $\Gamma(\lambda)$. Now values of λ are computed, say λ_3, which maximize this parabola. If the parabola has no maximum, λ_3 is set equal to λ_2. If $(\theta^{(0)} + \lambda_3\Delta\theta)$ is infeasible, λ_3 is truncated approximately. The following cases are considered:

(1) $\Gamma(\lambda_2) > \Gamma(0)$. If $\dfrac{\lambda_3\lambda_2}{\lambda_0} < 0.1$, set $\lambda = \lambda_2$ or $\lambda = \lambda_3$

and proceed to the next iteration depending upon whether $\Gamma(\lambda_2)$ is or is not greater than $\Gamma(\lambda_3)$.

(2) $\Gamma(\lambda_2) \leq \Gamma(0)$.

Set $\lambda_4 = \max(\lambda_3, \frac{1}{4}\lambda_2)$ and compute $\Gamma(\lambda_4)$. If $\Gamma(\lambda_4) > \Gamma(0)$ set $\lambda = \lambda_4$ proceed to next iteration. Otherwise replace λ_2 with λ_4, draw a parabola and proceed as before.

Convergence and Termination

In principle the method converges to a stationary point of the objective function, provided the latter possesses continuous first derivatives. The process is terminated when each component of the vector $\lambda\Delta\theta$ is so small as to satisfy the inequality:

$$|\lambda\Delta\theta_i \leq 0.0001\ (0.001 + |\theta_i^{(0)}|) \qquad (i=1,\ 2,\ \ldots,\ \ell)$$

(A-3.4.3)

This criterion was suggested by Marquardt (1963). However it does not guarantee that the amximum has been attained, but seems to work in most practical situations.

Penalty Functions

It was stated above that objective function must have continuous derivatives. When bounds or complex contraints are placed on θ the distribution function $p_0(\theta)$ may be discontinuous; that is it may be zero outside the acceptable region and finite inside it. Bard (1966) has suggested the following device to smooth out this discontinuity.

Suppose the restrictions placed on θ are stated in the form of inequalities:

$$Z_i(\theta) \leq 0 \qquad (k = 1,\ 2,\ \ldots,\ r) \qquad \text{(A-3.4.4)}$$

where the Z_i are specified functions. For instance, in the case of bounds $\alpha_i \leq \theta_i \leq \beta_i$ the corresponding Z_i would be:

$$Z_{2i-1}(\theta) = (\alpha_i - \theta_i) \leq 0 \tag{A-3.4.5}$$

$$Z_{2i}(\theta) = (\theta_i - \beta_i) \leq 0 \tag{A-3.4.6}$$

Now the prior distribution $p_o(\theta)$ is replaced by the function $p_o^*(\theta) = p_o(\theta) \exp \sum_{i=1} \frac{\nu_i}{Z_i(\theta)}$, where ν_i are preassigned constants. If ν_i are sufficiently small, p_o^* will not differ appreciably from p_o in the interior of the acceptable region, where Z_i are significantly different from zero. As one approaches the boundary of the region, however, at least one Z_i approaches zero from the negative side and hence p_o^* also approaches zero. Since p_o enters G through its logarithm, replacing p_o is equivalent to adding the penalty function $\sum_{i=1} \frac{\nu_i}{Z_i(\theta)}$ to $G(\theta)$, as suggested by Carroll (1961).

The maximization proceeds in several phases: first, the maximum of G and the penalty function is found. If at this point the value of penalty function is not negligible, the ν_i are multiplied by 0.1, and the maximum of the resulting function is found. If necessary, this process is repeated once more. Finally, the true maximum of G is found. If the maximum of G is an interior point of the admissible region, all the maxima will practically coincide. Letting

$$Z = \sum_{i=1}^{r} \frac{\nu_i}{Z_i(\theta)} \tag{A-3.4.7}$$

The required derivatives can be found by differentiation.

$$\frac{\partial Z}{\partial \theta_\alpha} = - \sum_{i=1}^{r} \frac{\nu_i}{Z_i^2(\theta)} \frac{\partial Z_i}{\partial \theta_\alpha} \tag{A-3.4.8}$$

$$\frac{\partial^2 Z}{\partial \theta_\alpha \partial \theta_\beta} = \sum_{i=1}^{r} \frac{\nu_i}{Z_i^3} [2 \frac{\partial Z_i}{\partial \theta_\alpha} \frac{\partial Z_i}{\partial \theta_\beta} - Z_i \frac{\partial^2 Z_i}{\partial \theta_\alpha \partial \theta_\beta}] \tag{A-3.4.9}$$

The important thing to note here is that when the constraints are linear (in particular, in the case of upper and lower bound), we have

$$\frac{\partial^2 Z_i}{\partial \theta_\alpha \partial \theta_\beta} = 0 \tag{A-3.4.10}$$

CHAPTER 4

EVALUATION OF METHODS TO ESTIMATE BOD PARAMETERS IN A TRANSIENT BOD MODEL FROM STOCHASTIC INPUT-OUTPUT DATA

4.1 INTRODUCTION

Mathematical models which adequately describe the water quality of polluted streams are essential in the assessment of water quality and in the determination of efficient management policies. In some instances the functional form of a model, and perhaps some of the parameters are known from theoretical analysis or previous tests. However, in almost all cases, complete specification of the model requires estimation of unknown parameters of the model based on experimental data.

Some investigators (Koivo and Phillips, 1972; Shastry et al., 1973) have proposed models in the form of ordinary differential equations to represent the river system under steady state conditions. However, these models are inadequate when significant changes in stream quality take place over time and space. The estimation of parameters in transient models is mathematically equivalent to the estimation of parameters in partial differential equations. Systems described by partial differential equations are generally referred to as Distributed Parameter Systems (D.P.S.).

The problem of estimating parameters in D.P.S. has been studied by many investigators in several fields of engineering (Seinfeld and Chen, 1971; Carpenter et al., 1971). To the best of the author's knowledge, there has been only one instance reported in the literature (Koivo and Phillips, 1971) where an attempt was made to estimate parameters in water quality models formulated in terms of partial differential equations. Koivo and Phillips (1971) successfully applied a stochastic algorithm to identify some of the unknown parameters in a transient model describing BOD and DO concentrations in polluted streams. A new approach to estimate parameters in a transient water quality model was presented in Chapter 3 of this dissertation. It was shown that the parameters appearing in the model equations can be estimated from experimental data collected at only two monitoring stations x_1 miles apart and using a minimum number of data points. Parameter estimates were obtained using Bard's method for parameter estimation.

The approach presented in Chapter 3 to estimate parameters for a system with noisy input is employed in this chapter. However, in this chapter the identification procedure is addressed to two systems and only BOD measurements (under isothermal conditions) are used. The first system represents the case when there exist random variations in BOD concentrations at the beginning of the stream section, due to changes in environmental conditions. The second system considered is a system with a noise-corrupted output (measurement noise). In addition, a gradient technique (Bard, 1967) and a Simplex search technique (Nelder and Mead, 1965) modified to take into account constraints in the parameters are used to identify some of the parameters appearing in the system equations. Parameter estimates obtained from these two methods are compared to evaluate the best method of estimation for the systems considered. Results are extended to a system with both noisy input and noise-corrupted output.

4.2 MATHEMATICAL MODEL

The mathematical model used in this study describes only the BOD concentrations in a polluted stream. The equation for the BOD profile along the stream is based on the following assumptions:

(1) The stream is under isothermal conditions.

(2) The cross sectional area of the stream is uniform.

(3) The velocity of the stream, u, is uniform.

(4) The rate process for BOD decay due to bacterial oxidation, k_1, and due to sedimentation, k_3, are both first order reactions; the rate being proportional to the amount of BOD present.

(5) The addition of BOD from the local runoff, L_a, is uniform along the stream.

Under these assumptions, the temporal and spatial distribution of BOD may be written as follows:

$$\frac{\partial L}{\partial t} + u\frac{\partial L}{\partial x} + (k_1 + k_3)L - L_a = 0 \tag{4.1}$$

where

L = BOD concentration.

Subject to

$$\frac{\partial L}{\partial t} = 0 \quad \text{at } t = 0^-,\ x > 0 \tag{4.2}$$

$$L = L_0 \quad \text{at } t \leq 0^-,\ x > 0 \tag{4.3a}$$

$$L = L(t) \text{ at } x = 0^+,\quad t \geq 0 \tag{4.3b}$$

Equation (4.2) indicates that initially ($t = 0$) the BOD profile is at the steady state condition. At $t = 0^+$, there is a waste discharge into the stream at $x = 0$ which disturbs the system. Assuming instantaneous mixing of the waste with the stream flow, the BOD concentration immediately following the mixing point is given by equation (4.3).

Equation (4.1) is a linear first-order partial differential equation which readily submits to the method of characteristics (Abbot, 1966). The direct application of the method of characteristics to equation (4.1) gives

$$\frac{dx}{dt} = u \tag{4.4}$$

$$\frac{dL}{dt} = -(k_1 + k_3)L + L_a \tag{4.5}$$

The solution of equations (4.4) and (4.5) is divided into two parts depending upon the selection of the boundary conditions. The initial steady state is obtained if the initial condition is chosen along the $t = 0$ axis, i.e., $0 \leq t \leq x/u$. The response of the system to the waste discharge at $x = 0^+$ is obtained if the initial condition is chosen along the $x = 0$ axis ($t \geq x_1/u$). Details of the analytical solution are given in Appendix 4.1. The complete solution is given below.

(a) Initial condition along the $t = 0$ axis: $0 \leq t \leq x/u$ ($x \geq ut$)

$$L(x,t) = L(x - ut,0)e^{-(k_1 + k_3)t} - \frac{L_a}{k_1 + k_3}[1 - e^{-(k_1 + k_3)t}] \tag{4.6}$$

(b) Initial condition along the x = 0 axis: $t \geq x/u$ $(0 \leq x \leq ut)$

$$L(x,t) = L(0^{+},t - x/u)e^{-(k_1 + k_3)x/u} - \frac{L_a}{k_1 + k_3}[1 - e^{-(k_1 + k_3)x/u}] \quad (4.7)$$

The function $L(0,t - x/u)$ can be any arbitrary function of time. Figure (4.1) shows the BOD distribution due to a step input of waste at the point x=0 starting at t = 0.

Two quantities are correlated when they exhibit behavior patterns at the same time, or with some time lag between them. BOD data, when measured at two monitoring stations x_1 miles apart, are good examples of events that are correlated at different times. If a suitable time lag ($\tau = x_1/u$) is used, the observations from the two stations will correlate well; but for other time lags the correlation will be poor.

Equation (4.7) shows that the BOD values measured at $x = 0^{+}$ (after mixing) can be correlated with BOD values measured at $x = x_1$ after the time lag $\tau = x_1/u$ (input-output type of data). Therefore, parameters appearing in equation (4.1) may be estimated from experimental data collected at only two locations using equation (4.7) as the correlation equation. A minimum number of data points is needed since as few as two pairs of input-output data points are enough to draw the straight line represented by equation (4.7).

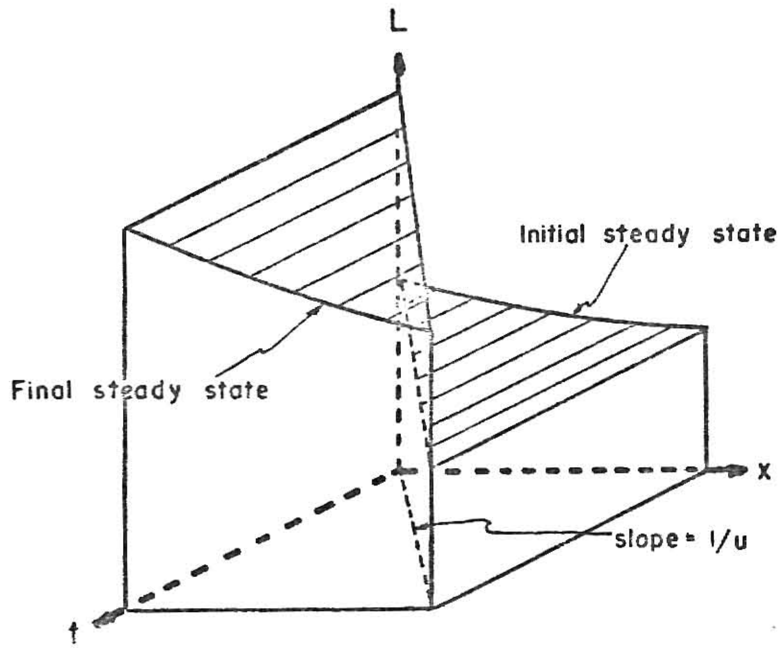


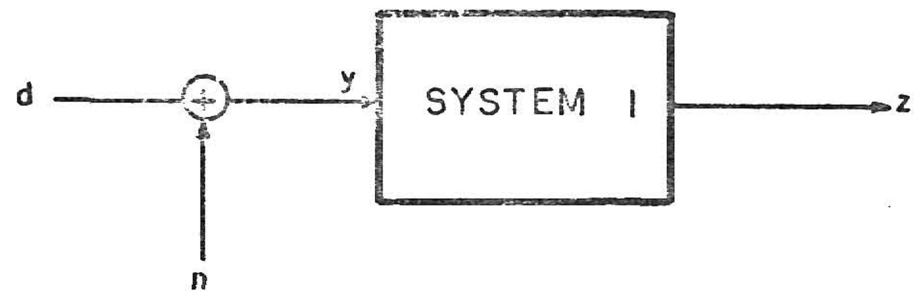
Fig. 4.1 Response of stream BOD subject to a waste discharge (step change)

4.3 PROBLEM STATEMENT

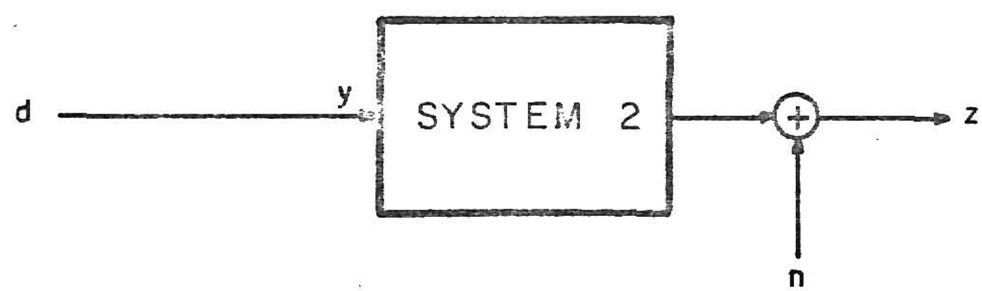
Two different systems are studied (see Fig. 4.2). A section of a river stream of length x_1, with a single waste discharge, is considered in both systems. The section starts just below the waste discharge at $x = 0^+$. In System 1, the BOD concentration changes randomly at the inlet ($x = 0^+$) and these variations are transmitted through the system. Such a situation often occurs in real systems when stream conditions are affected by local weather conditions. The changes at $x = 0^+$ are assumed to be made up of a deterministic component d(t), and a stochastic component n(t). In System 2, the stochastic component n(t) (white noise) is added to the output to simulate data with measurement error. This situation is also found in real systems. Both systems can be described by equation (4.1). The analytical solution of equation (4.1) for $t \geq x_1/u$ can be used to correlate input-output data for both systems. This solution is given by equation (4.7).

The parameters appearing in equation (4.7) are L_a, k_1 and k_3. Let us assume that L_a is known, then only k_1 and k_3 are to be determined. It can be observed that k_1 and k_3 appear as the sum $(k_1 + k_3)$ in equation (4.7). It was noted in Chapter 3 that these parameters must be combined as a single parameter k_r ($k_r = k_1 + k_3$) when only BOD data are used for parameter estimation. This is due to the fact that k_1 cannot be determined independently of k_3.

The value of $\tau = x_1/u$, the time lag of the system, is needed to correlate input-output data. In most cases, the value of x_1 may be



System 1. Noisy input



System 2. Noisy measurements

Fig. 4.2 Systems used for parameter identification determined without excessive error but u is generally not accurately known. Due to this uncertainty in the value of u, we may choose to consider τ as an additional parameter. It is likely that a good estimate of τ is available. In this case τ need not be considered as an additional parameter. In this study, τ is considered as a parameter.

The estimation problem can be stated as the estimation of the parameters k_r and τ in such a way that equation (4.7) fits the input-output data when plotted on a scatter diagram. This diagram may be constructed by plotting paired observations of BOD measured at $x = 0^+$ (input variable) and at $x = x_1$ (output variable). In this diagram, the output variable is plotted as a function of the input variable.

4.4 CRITERION FUNCTION AND METHODS FOR ESTIMATION

In any parameter estimation problem, a criterion is needed to measure the accuracy of the parameter estimates. The most widely used criterion is the standard least squares criterion. The parameter estimates can be determined by minimizing the least squares criterion function given below which represent the deviation of the predicted output BOD values from the measured output BOD values.

$$\min_{\{k_r, \tau\}} S = \min_{\{k_r, \tau\}} \sum_{n=1}^{N} \left[L(x_1, t_n)_{measured} - L(x_1, t_n)_{predicted}\right]^2 \tag{4.8}$$

Here, k_r and τ are the parameters to be estimated. As stated in Section 4.3, these parameters can be estimated in such a way that equation (4.7) fits the measured input-output BOD data on a scatter diagram.

Equation (4.7) is nonlinear with respect to the parameters k_r and τ. Several techniques are available to estimate parameters in nonlinear models (Gauss, 1957; Bard, 1967; Nelder and Mead, 1965). Bard's method and a Simplex search technique modified to take into account constraints in the parameters are used in this work to minimize the least square criterion function given by equation (4.8). Bard's method involves two steps. First, a steepest descent algorithm is used in the initial iterations and for the final iterations linearization techniques are applied. On the other hand, the Simplex method does not require the evaluation of derivatives as in Bard's method and is fairly simple to use. A brief description of the Simplex method is presented in Appendix 4.2. A description of Bard's method was given in Chapter 3 (see Appendix 3.4) and is not presented here.

4.5 COMPUTATIONAL PROCEDURE

Equation (4.7) was used to generate the output data for parameter estimation. The deterministic signal used for both systems (at $x = 0^+$) was a cyclic signal with a period of 365 days which represents yearly variations of BOD concentrations. The signal is given by the function

$$d(t) = 15.0 + 5.0 \sin (2\pi t/365), \text{ ppm.}$$

This cyclic function gave a reasonable spread in the data which was essential in correlating input-output BOD data. The stochastic signal for System 1 and the noise added in System 2 were represented by normally distributed random numbers. These normally distributed random numbers were generated by using the scientific subroutine

GAUSS (IBM, 1966). Four values of standard deviations, σ, viz., 10^{-4}, 10^{-3}, 10^{-2}, and 10^{-1} were used. The procedure adopted in both systems is given below.

(1) Find parameters k_r and τ in equation (4.7) using Bard's method.

(2) Find parameters k_r and τ in equation (4.7) using the modified Simplex search technique and compare the parameter estimates with the estimates obtained in (1).

(3) Compare the values of the criterion functions obtained from (1) and (2). In addition, compare the number of function evaluation and the execution time required to obtain the parameter estimates.

The fast core of an IBM 360/50 Digital Computer was used to perform the simulation and calculations. Computer programs were available to estimate the parameters k_r and τ. The programs required slight modifications and were fairly efficient from the computational standpoint. The values of the parameters used in the simulation were L_a = 0.20 ppm/day, $k_r = k_1 + k_3$ = 0.36 1/day (k_1 = 0.16 1/day; k_3 = 0.20 1/day), and τ = 1 day. The values of L_a, k_1 and k_3 are typical values for Kansas rivers (Fan et al., 1972). The initial estimates used for the iterative procedure were arbitrarily chosen for both systems.

4.6 RESULTS

The computational results for System 1 are presented in Tables 4.1 through 4.5. In Tables 4.1 through 4.4, Column (1) gives the estimated parameters, Columns (2) and (3) show, respectively, the final estimates

Table 4.1 Estimated Values of Parameter for $\sigma = 10^{-4}$

System 1

Parameter (1)	Bard's Method: Final Estimates (2)	Bard's Method: Standard Deviation (3)	Simplex Method: Final Estimates (4)
k_r	0.359991	0.0	0.319692
τ	0.100001×10^{1}	0.0	0.113207×10^{1}

Table 4.2 Estimated Values of Parameter for $\sigma = 10^{-3}$

System 1

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.359996	0.1274×10^{-5}	0.379885
τ	0.999996	0.3690×10^{-5}	0.945541

Table 4.3 Estimated Values of Parameter for $\sigma = 10^{-2}$

System 1

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.359991	0.7173×10^{-5}	0.315982
τ	0.100001×10^{1}	0.2077×10^{-4}	0.114617×10^{1}

Table 4.4 Estimated Values of Parameter for $\sigma = 10^{-1}$

System 1

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.359992	0.0	0.279891
τ	0.100001×10^1	0.0	0.130220×10^1

Table 4.5 Other Estimates Used for Evaluation of the Methods

System 1

	Bard's Method			Simplex Method		
Standard Deviation, σ (1)	Criterion Function (2)	Function Evaluations (3)	Execution Time* (4)	Criterion Function (5)	Function Evaluations (6)	Execution Time* (7)
10^{-4}	0.0	36		0.3067×10^{-4}	32	
10^{-3}	0.9095×10^{-12}	23		0.4878×10^{-5}	33	
10^{-2}	0.2546×10^{-10}	42		0.3667×10^{-4}	37	
10^{-1}	0.0	41	1.86 min	0.1600×10^{-3}	34	1.14 min

*Total execution time for four values of σ.

and standard deviation of the parameters obtained by Bard's method, and Column (4) gives the final estimates of the parameters obtained from the Simplex method. Table 4.5 shows the minimum values of the function S [see equation (4.8)], the number of function evaluations and the execution time required by Bard's method and the Simplex method to obtain the final estimates of the parameters. Figures 4.3 and 4.4 show, respectively, k_r and τ as functions of the standard deviation, σ. Figure 4.5 illustrates the minimum values of the function S as functions of σ.

Tables 4.6 through 4.11 show the results for System 2. The parameter estimates obtained by Bard's method and the Simplex method are presented in Tables 4.6 through 4.10. Table 4.11 shows the other estimates used to compare the two methods employed to estimate the parameters in this system. The results for System 2 are illustrated in Figs. 4.6 through 4.8. The parameters k_r and τ are shown in Figs. 4.6 and 4.7, respectively. The solid line in these figures represents the nominal value of the parameters. The minimum values of the function S [see equation (4.8)] are illustrated in Fig. 4.8.

4.7 ANALYSIS AND DISCUSSION

An inspection of Tables 4.1 through 4.10 and Figs. 4.3 through 4.8 reveals that the parameter estimates deviate from their nominal values as expected. For the purpose of comparision the deviations for each parameter were computed as percentage deviations from their nominal or actual values. Table 4.11 shows the percentage deviations for System 1 and Table 4.12 the percentage deviations for System 2. It can be seen from these tables that the parameter estimates deviate depending upon

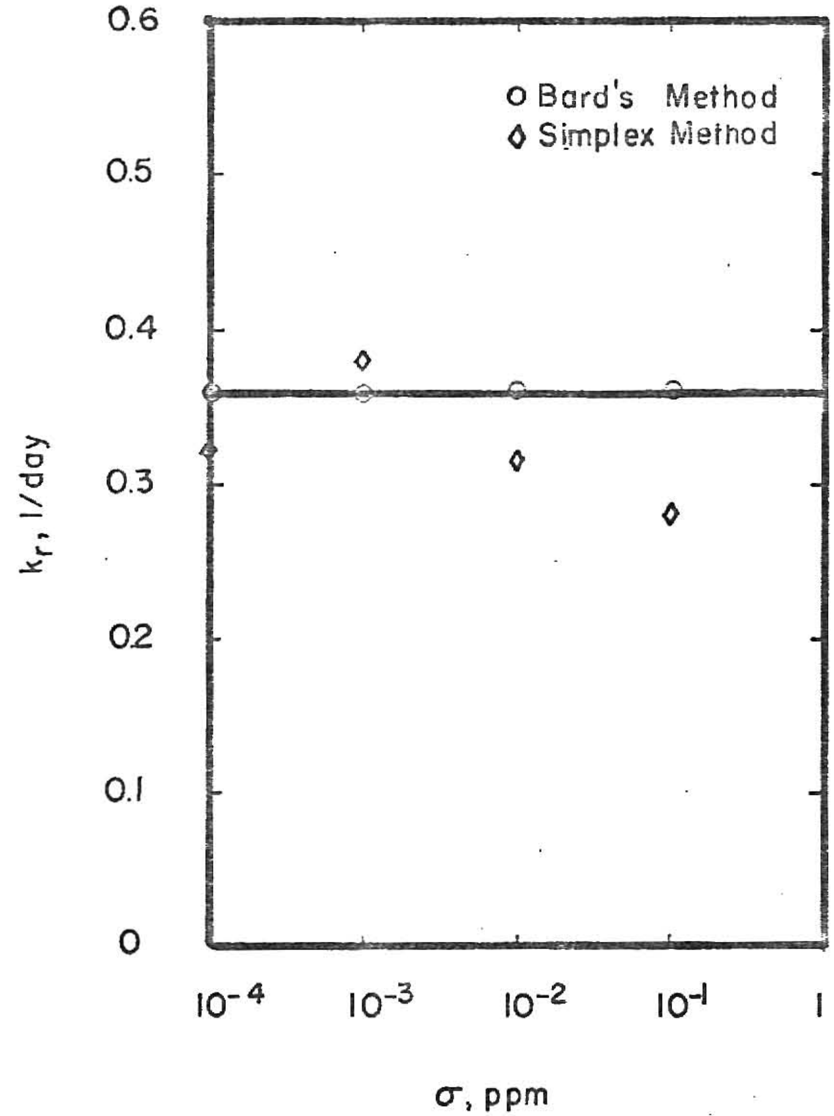


Fig. 4.3 Estimated values of k_r as a function of σ for System I

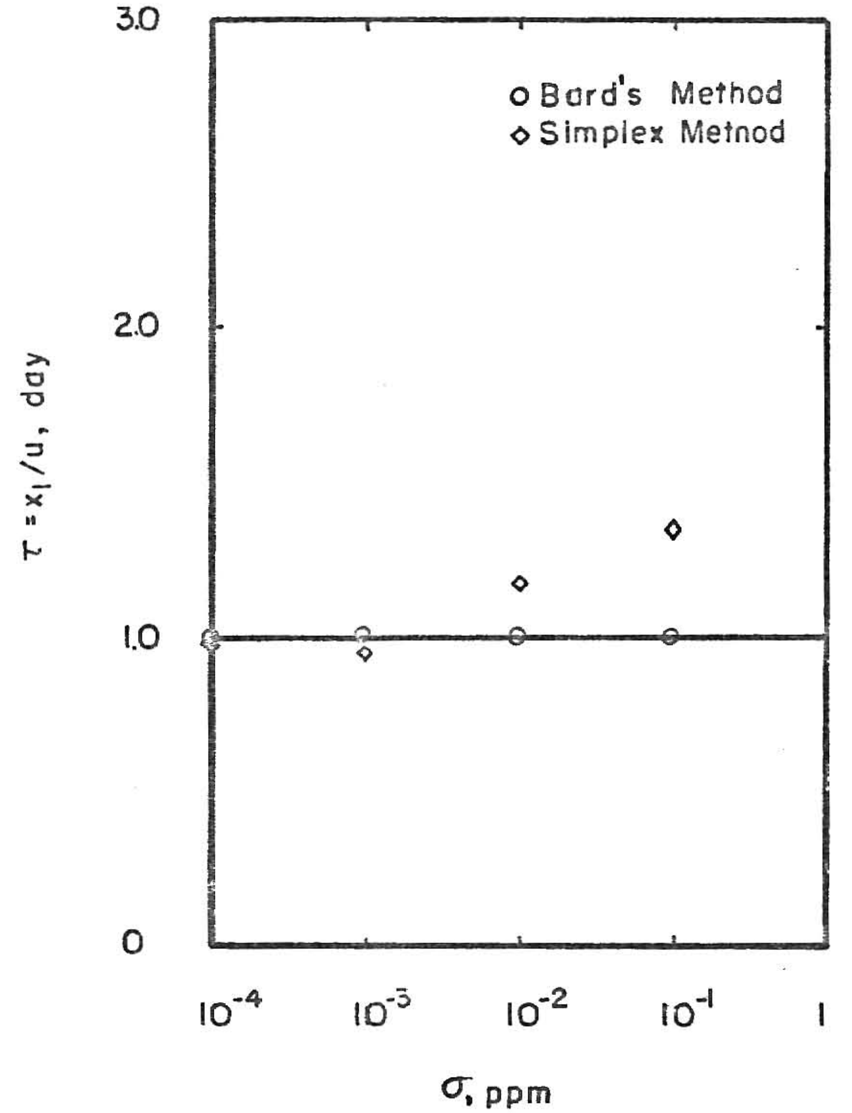


Fig. 4.4 Estimated values of τ as a function of σ for System I

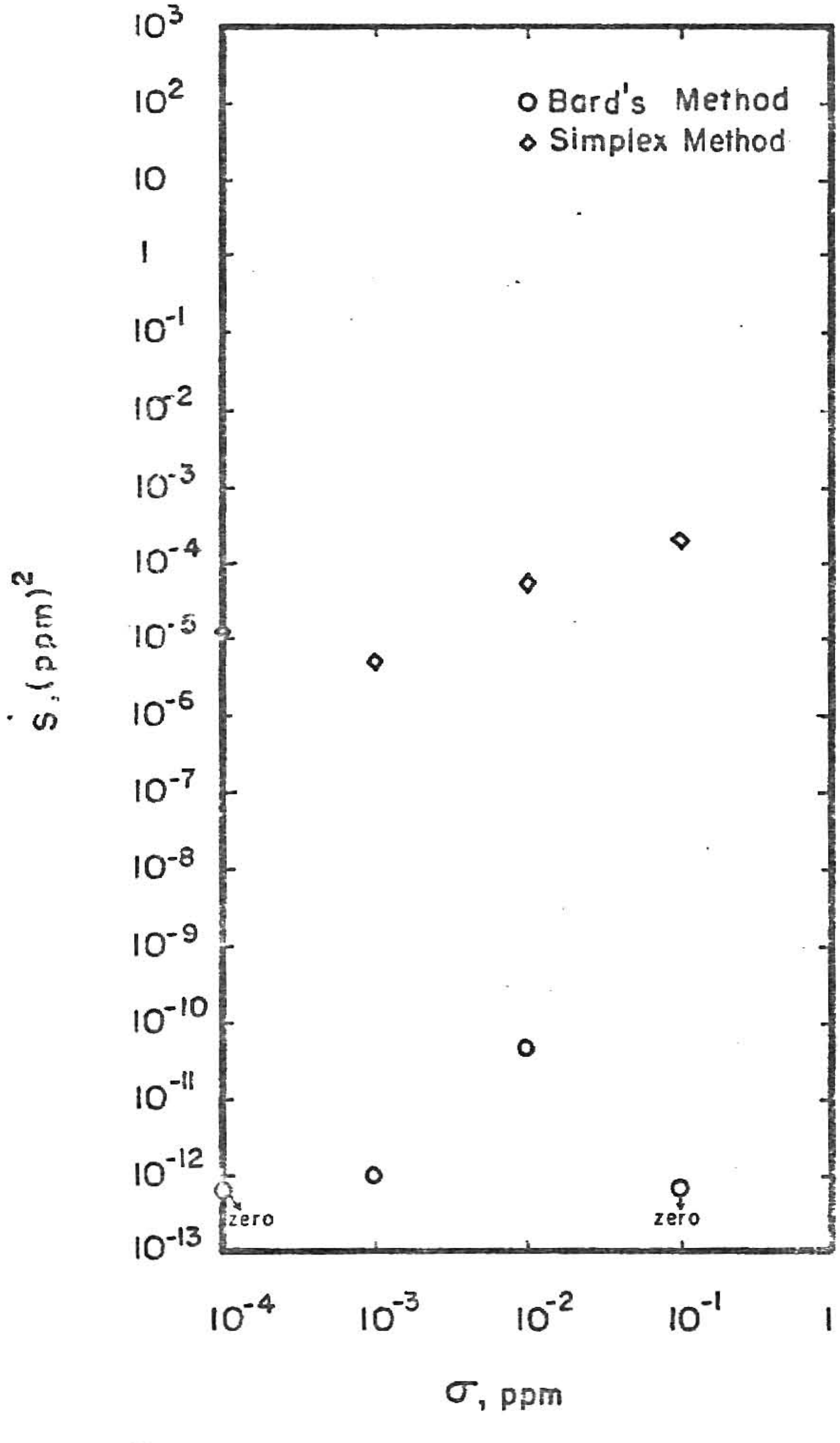


Fig. 4.5 Estimated values of S as a function of σ for System I

Table 4.6 Estimated Values of Parameter for $\sigma = 10^{-4}$

System 2

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.360047	0.9587×10^{-3}	0.319692
τ	0.999851	0.2776×10^{-2}	0.113207×10^{1}

Table 4.7 Estimated Values of Parameter for $\sigma = 10^{-3}$

System 2

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.371679	0.7595×10^{-2}	0.379885
τ	0.967241	0.2058×10^{-1}	0.945541

Table 4.8 Estimated Values of Parameter for $\sigma = 10^{-2}$

System 2

Parameter (1)	Bard's Method Final Estimates (2)	Bard's Method Standard Deviation (3)	Simplex Method Final Estimates (4)
k_r	0.284858	0.4405×10^{-1}	0.315639
τ	0.127891×10^{1}	0.2086	0.114820×10^{1}

Table 4.9 Estimated Values of Parameter for $\sigma = 10^{-1}$

System 2

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.746933×10^{-1}	0.2307×10^{-1}	0.280770
τ	0.577127×10^{1}	0.2222×10^{1}	0.130044×10^{1}

Table 4.10 Other Estimates Used for Evaluation of the Methods

System 2

	Bard's Method			Simplex Method		
Standard Deviation, σ (1)	Criterion Function (2)	Function Evaluations (3)	Execution Time* (4)	Criterion Function (5)	Function Evaluations (6)	Execution Time* (7)
10^{-4}	0.3712×10^{-6}	63		0.3137×10^{-4}	32	
10^{-3}	0.2462×10^{-4}	34		0.2576×10^{-4}	33	
10^{-2}	0.1976×10^{-2}	33		0.2008×10^{-2}	37	
10^{-1}	0.1941	61	1.98 min	0.2245	37	1.32 min

*Total execution time for four values of σ

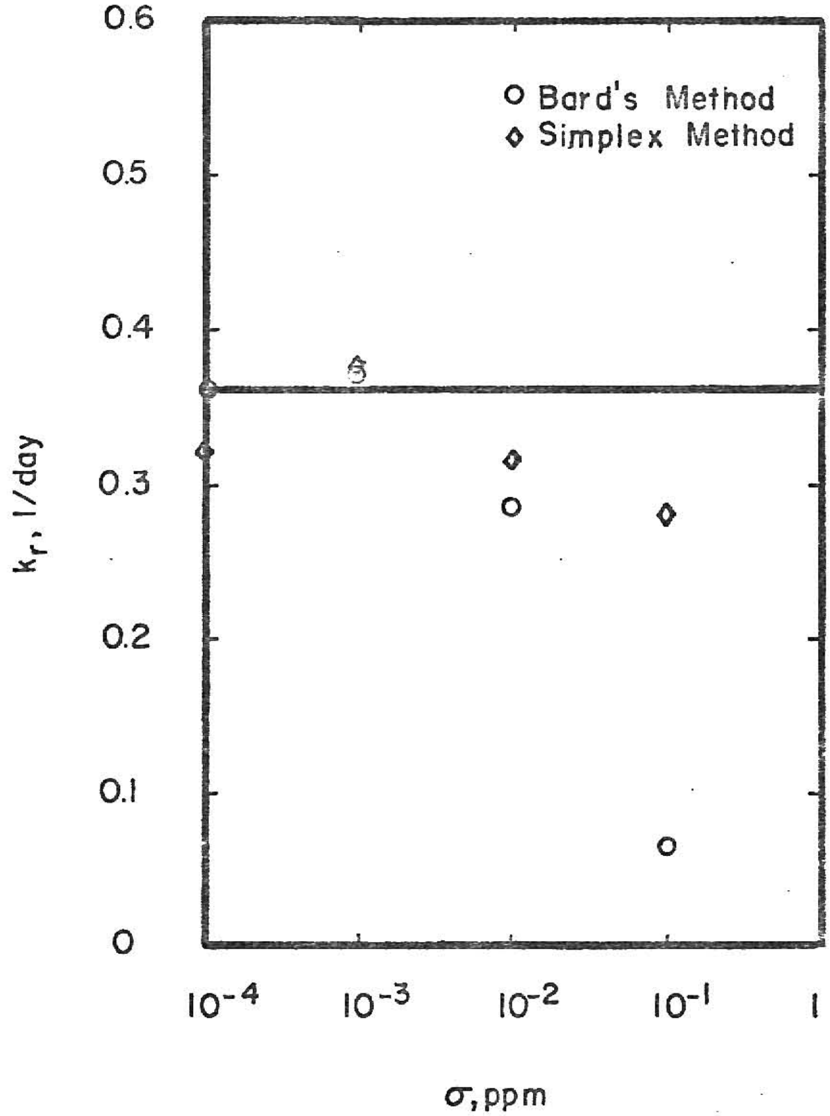


Fig. 4.6 Estimated values of k_r as a function of σ for System 2

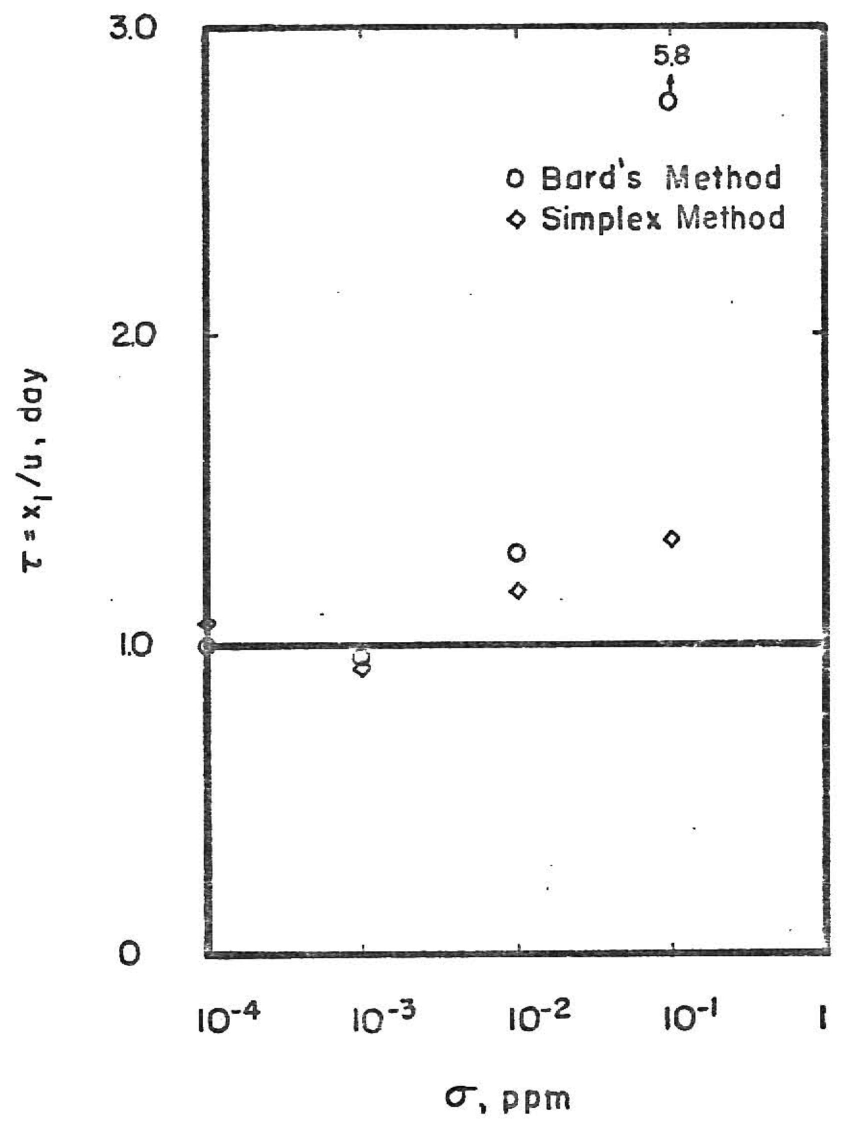


Fig. 4.7 Estimated values of τ as a function of σ for System 2

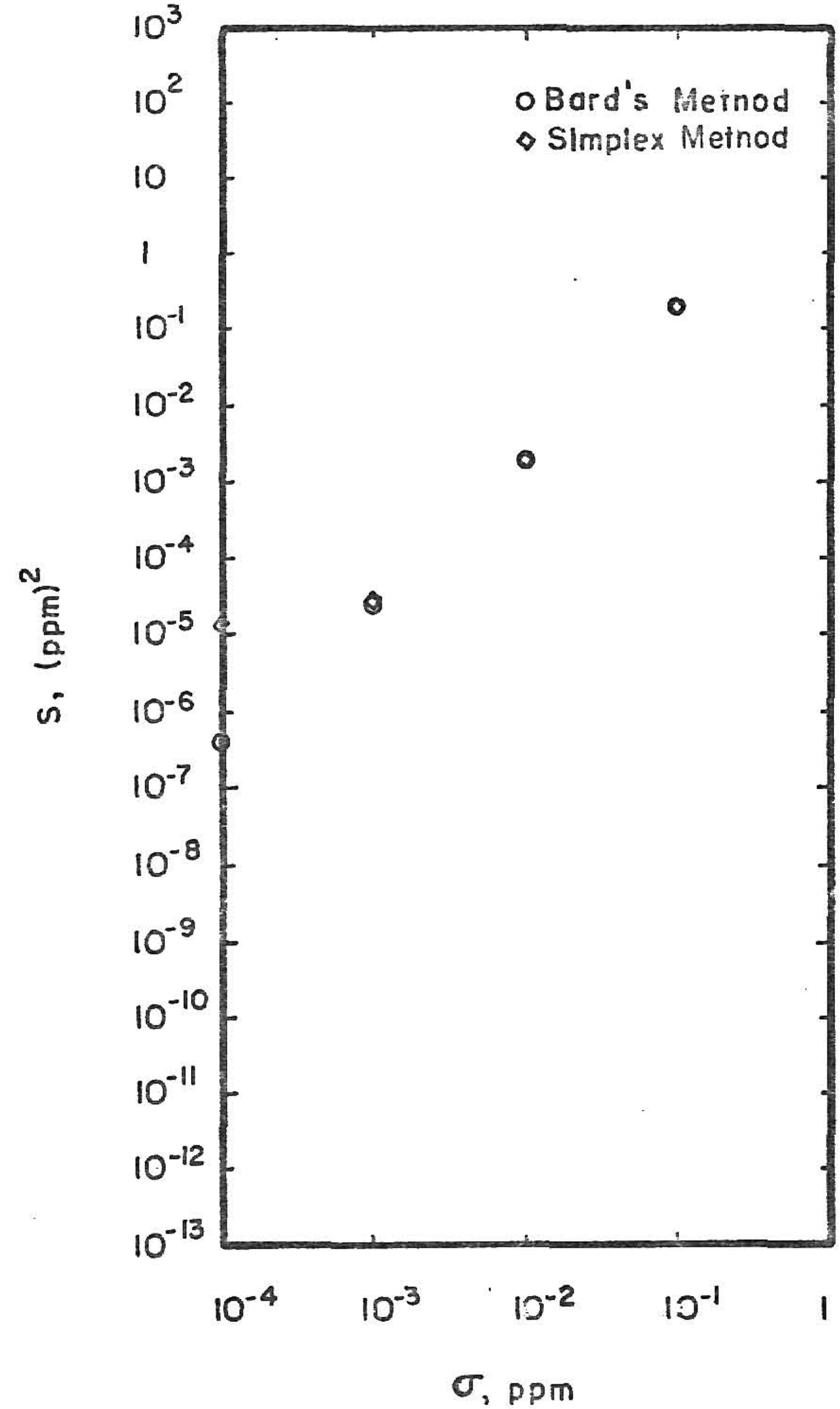


Fig. 4.8 Estimated values of S as a function of σ for System 2

Table 4.11 Deviation Percentages of Parameters from their Actual Values

System 1

Parameter	Bard's Method				Simplex			
	Standard Deviation, σ				Standard Deviation, σ			
	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
k_r	-10^{-3}	-10^{-3}	-10^{-3}	-10^{-3}	-11	+ 5	-12	-22
τ	$+10^{-3}$	-10^{-3}	$+10^{-3}$	$+10^{-3}$	+13	- 5	+14	+30

Table 4.12 Deviation Percentages of Parameters from their Actual Values

System 2

Parameter	Bard's Method				Simplex			
	Standard Deviation, σ				Standard Deviation, σ			
	10^{-4}	10^{-3}	10^{-2}	10^{-1}	10^{-4}	10^{-3}	10^{-2}	10^{-1}
k_r	$+10^{-2}$	+ 3	-20	-78	-11	+ 5	-12	-22
τ	-10^{-2}	- 3	+27	>+100	+13	- 5	+14	+30

the type of measurement data used and on the technique employed to estimate the parameters k_r and τ. Therefore, it is convenient to analyze the deviations for each system separately. This is done in order to select the best method for parameter estimation according to the type of data used for the estimation procedure.

System 1. Each method of estimation was applied to the same experimental data obtained for System 1 to estimate the parameters k_r and τ. It is known from Chapter 3, that for conditions similar to the conditions used in System 1 the standard deviation σ of the noisy input signal contributed very little to the deviations of the parameter estimates. This can be observed in Table 4.11 for Bard's method. However, the use of the Simplex method leads to deviations of the parameter estimates which are significantly higher compared to the results from Bard's method (see Table 4.11 and Figs. 4.3 and 4.4). From Table 4.5, it can be seen that there are no significant differences between the two methods as far as number of function evaluations is concerned. In addition, the values of the criterion function S computed by Bard's method are better than the values obtained with the Simplex method (see also Fig. 4.5), and the computational time involved in the estimation of parameters for all four values of σ is substantially smaller for the Simplex method than for Bard's method since the latter required evaluation of derivatives with respect to the parameters.

From the results obtained for System 1, Bard's method is recommended for obtaining the parameters of a system with noisy input since it gave definitely better estimates of the parameters than the Simplex method.

System 2. This system represented the case in which output data measured at $x = x_1$ were noise-corrupted. The parameter estimates should diverge, in general, from the nominal values of the parameters, as the standard deviation σ of the introduced error increases. This divergence is apparent from the results obtained for System 2 (see Tables 4.6 through 4.9 and Figs. 4.6 and 4.7). A comparison of the deviation of the parameters estimated by the two methods shows that for values of σ greater than 10^{-3} the Simplex method gives better estimates than Bard's method. The situation was reversed when the values of σ were equal to or less than 10^{-3} (see Table 4.12). It can seen from Table 4.10 that the estimated values of the criterion function S given by Bard's method are similar to the values given by the Simplex method for σ greater than or equal to 10^{-3}; the number of functions evaluated by the Simplex is smaller than the number of functions evaluated by Bard's method, and the computational times involved in the Simplex method and Bard's method are roughly in the ratio of 2 to 3.

From the results obtained for System 2, the Simplex search seems to be the method of choice to estimate the parameters k_r and τ. The main advantage of using the Simplex method is the fact that it is based neither on gradients (first-order derivatives, as in Bard's method) nor on quadratic forms (second-order derivatives). In addition, the level of the corrupting noise in actual field data is usually of the order of 10^{-1} which is well within the range of noise level tolerated by the Simplex search.

It is worth noting that L(0,t), the input signal of the system, can be any arbitrary function of time. It can be a deterministic signal, a stochastic signal, or a combination of both. If parameters were to be estimated for a system (System 3) with a stochastic input as is System 1 and with noisy measurements as in System 2, the results of parameter estimation would be similar to the results obtained for System 2. This can be visualized as follows. For the constant parameter linear system used in this study, no information is lost or hidden in the output signal for any input. What is most important to the estimation procedure is the level of the noise added to the output signal since the information on the actual output signal is hidden by the level of the corrupting noise (as in System 2). Parameters were estimated for System 3 and the results obtained were in agreement with the results expected. The results for System 3 are presented in Appendix 4.3.

4.8 CONCLUSION

A gradient method (Bard, 1967) and a Simplex search technique (Nelder and Mead, 1965) were used to estimate BOD parameters for several systems. The time-lag phenomenon was used to correlate input-output data. For a system with noisy input (System 1), Bard's method seems to be the method of choice to estimate k_r and τ, whereas for a system with noise added to the output signal (System 2) the Simplex method seems to be the method of choice. The level of the noise added to the output signal of the system is the important factor is estimating parameters. It is suggested that the DO parameters be estimated following the same procedure used in theis chapter. The same approach may be used to estimate parameters in linear distributed parameter systems. Such systems are representative of a large class of systems in chemical engineering, and other disciplines.

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APPENDIX 4.1

ANALYTICAL SOLUTION OF THE BOD EQUATION BY THE METHOD OF CHARACTERISTICS (Abbot, 1966)

To solve equation (4.1) it is assumed that its region of integration is a space of three dimensions, with coordinates t, x, L. Treating L as the dependent variable, with t and x independent, we then have two "principal slopes": $\partial L/\partial t$ in the t direction, and $\partial L/\partial x$ in the x direction. These two slopes together define the increment dL in terms of the increment dt and dx, by

$$\frac{\partial L}{\partial x} dt + \frac{\partial L}{\partial x} dx = dL \qquad \text{(A-4.1.1)}$$

Let us rearrange equation (3.1) and write it as

$$\frac{\partial L}{\partial t} (1) + \frac{\partial L}{\partial x} (u) = [-(k_1+k_3)L+L_a] \qquad \text{(A-4.1.2)}$$

Treating (A-4.1.1) abd (A-4.1.2) as a pair of simultaneous equations for $\partial L/\partial t$ and $\partial L/\partial x$, a set of planar elements may be defined. Equations (A-4.1.1) and (A.4.1.2) can be written in vector form as

$$\begin{vmatrix} 1 & u \\ dt & dx \end{vmatrix} \begin{vmatrix} \partial L/\partial t \\ \partial L/\partial x \end{vmatrix} = \begin{vmatrix} -(k_1+k_3)L+L_a \\ dL \end{vmatrix} \qquad \text{(A-4.1.3)}$$

If they are linearly dependent the following relationships must be satisfied

$$\begin{vmatrix} 1 & u \\ dt & dx \end{vmatrix} = 0 \qquad \text{(A-4.1.4)}$$

$$\begin{vmatrix} 1 & [-(k_1+k_3)L+L_a] \\ dt & dL \end{vmatrix} = 0 \tag{A-4.1.5}$$

and

$$\begin{vmatrix} [-(k_1+k_3)L+L_a] & u \\ dL & dx \end{vmatrix} = 0 \tag{A-4.1.6}$$

Solution of (A.4.1.4) - (A-4.1.6) give

$$\frac{dt}{1} = \frac{dx}{u} = \frac{dL}{-(k_1+k_3)L+L_a} \tag{A-4.1.7}$$

Equation (A-4.1.7) represents the line which is common to all the planar elements. This is the characteristic line. The slope of the base characteristic is given by

$$\frac{dx}{dt} = u \tag{A-4.1.8}$$

Equation (A-4.1.8) is the characteristic line (equivalent to equation (4.2) in Chapter 3) along which

$$\frac{dL}{dt} = -(k_1+k_3)L+L_a \tag{A-4.1.9}$$

is integrated. Equation (A-4.1.9) is equivalent (4.3) in Chapter 3.

The solution of equation (A-4.1.8) is given by

$$x - x_o = (t - t_o)u \tag{A-4.1.10}$$

and the general solution to the partial differential equation (4.1) is given be

$$L(x,t) = L(x_o,t_o)e^{-(k_1+k_3)(t-t_o)} + \frac{L_a}{k_1+k_3}(1-e^{-(k_1+k_3)(t-t_o)}) \quad \text{(A-4.1.11)}$$

(1) Initial condition along the t=0 axis, with $t_o=0$, $0 \leq t \leq x/u$

$$x_o = x - ut$$

and

$$L(x,t) = L(x-ut,0)e^{-(k_1+k_3)t} + \frac{L_a}{k_1+k_3}(1-e^{-(k_1+k_3)t}) \quad \text{(A-4.1.12)}$$

(2) Initial condition along the x=0 axis, with $x_o=0$, $t \geq x/u$

$$t_o = t - x/u$$

and

$$L(x,t) = L(0,t-x/u)e^{-(k_1+k_3)x/u} + \frac{L_a}{k_1+k_3}(1-e^{-(k_1+k_3)x/u}) \quad \text{(A-4.1.13)}$$

in which L(0, t-x/u) is any arbitrary function of t. Equation (A.4.1.12) represents the initial steady state and (A-4.1.13) the final steady state when a waste is dumped at t=0 and x=0. If so, L(0, t-x/u) is the BOD concentration after mixing.

APPENDIX 4.2

SIMPLEX PATTERN SEARCH TECHNIQUE FOR ESTIMATION OF PARAMETERS

The purpose of various parameter estimation techniques and search techniques is to minimize the selected criterion function. This criterion function is a measure of the difference between the measured experimental value of the response at particular values of the independent variable and the predicted response (from the mathematical model) based on the values of independent variables and parameters. The linearization techniques are based on the particular form of the convertional sum of squares criterion function with the assumption that the linearity assumption around the minimum criterion function value allows efficient progress. Sometimes for some non-linear models and for poor initial estimates of parameters the usual parameter estimation techniques like Guass method (Gauss, 1957) and Bard's modification (Bard, 1967) may be quite inefficient. Hence, here a search technique developed to minimize an objective function can be used.

The pattern search techniques are efficient and simple to use because they do not require derivatives. The Simplex method (Nelder and Mead, 1965), Box method (Box, 1965) and Hooke-Jeeves method (Hooke and Jeeves, 1961) are commonly used methods of this type. The particular method proposed be Nelder and Mead (1965) will be descirbed here briefly. A simplified description of the same can be found in the paper by Fan et al. (1969). To use this method for the minimization of a function of n variables, it is necessary to set up a Simplex of (n+1) vertices, that is, to select (n+1) trial points in n-dimensional space. The values of the objective function are then calculated at each of these points. By comparing the objective function value of these (n+1) points, the point with the highest value is replaced by a point with a lower value of the objective function. A lower function value if selected by a reflection, expansion or contraction operation through the centroid of the current Simplex. If none of these operations are successful, the Simplex is reduced is size around the lowest functional value before starting the next iteration.

For a two-dimensional problem where the objective function $y = f(x_1, x_2)$ is to be minimized, a Simplex with $(n+1) = 3$ points is required. Let P_1', P_2' and P_3' be three trial points, such that $y_1 < y_2 < y_3$, where

y_1 = objective function value at point 1

y_2 = objective function value at point 2

y_3 = objective function value at point 3

The various operations to get a point with lower objective function value are defined as

Reflection: $P_5' = P_4' + \alpha(P_4' - P_3')$ (A-4.2.1)

Expansion: $P_6' = P_4' + \eta(P_5' - P_4')$ (A-4.2.2)

Contraction: $P_7' = P_4' + \gamma(P_3' - P_4')$ (A-4.2.3)

where

P_4' = centroid of points P_1' and P_2', in general the centroid of a set of n points in a simplex is

$$P'_c = \sum_{i=1}^{n} (P_i/n) \qquad (A-4.2.4)$$

P'_5 = reflection of the point P'_3 with respect to P'_4

P'_6 = expansion of P'_5

P'_7 = contraction of the highest valued point P'_3 with respect to P'_4

The values of the coefficients, α, η and γ, considered best by Nelder and Mead (1965) are

$$\alpha = 1, \; \eta = \frac{1}{2}, \text{ and } \gamma = 2$$

However the best values of these coefficients may be different for different problems and should be found by experience. The details of the procedure have been given by Fan et al. (1969).

One stopping criterion is the occurrence of five consecutive values of the objective function which are considered "equal". Another stopping criterion would be to compare the "standard error" of the y's in the form

$$\left[\sum_{i=1}^{n+1} (y_i - \bar{y}) /n \right]^{1/2} \qquad (A-4.2.5)$$

with a preset value and stop the program when it falls below this value. The stopping criterion used for convergence in Chapter 4, is

$$\left[\sum_{i=1}^{n+1} (y_i - \bar{y}) /n \right]^{1/2} < 10^{-6} \qquad (A-4.2.6)$$

The success in employing the criterion for stopping computations depends upon the simplex not becoming too small in relation to the curvature of the surface as the final minimum is reached. The reasoning behind this criterion is given by Nelder and Mead (1965). They have suggested that in statistical problems where one is concerned with finding the minimum of a negative likelihood, the curvature near the minimum gives the information on unknown parameters. If the curvature is slight, the sampling variance of the estimates will be large and there is no sense in finding the co-ordinate of the minimum very accurately, while, if the curvature is very large, there is justification for pinning down the minimum more exactly.

Figure (A-4.2.1) shows the flow diagram given by Fan et al. (1969) for the Simplex pattern search method.

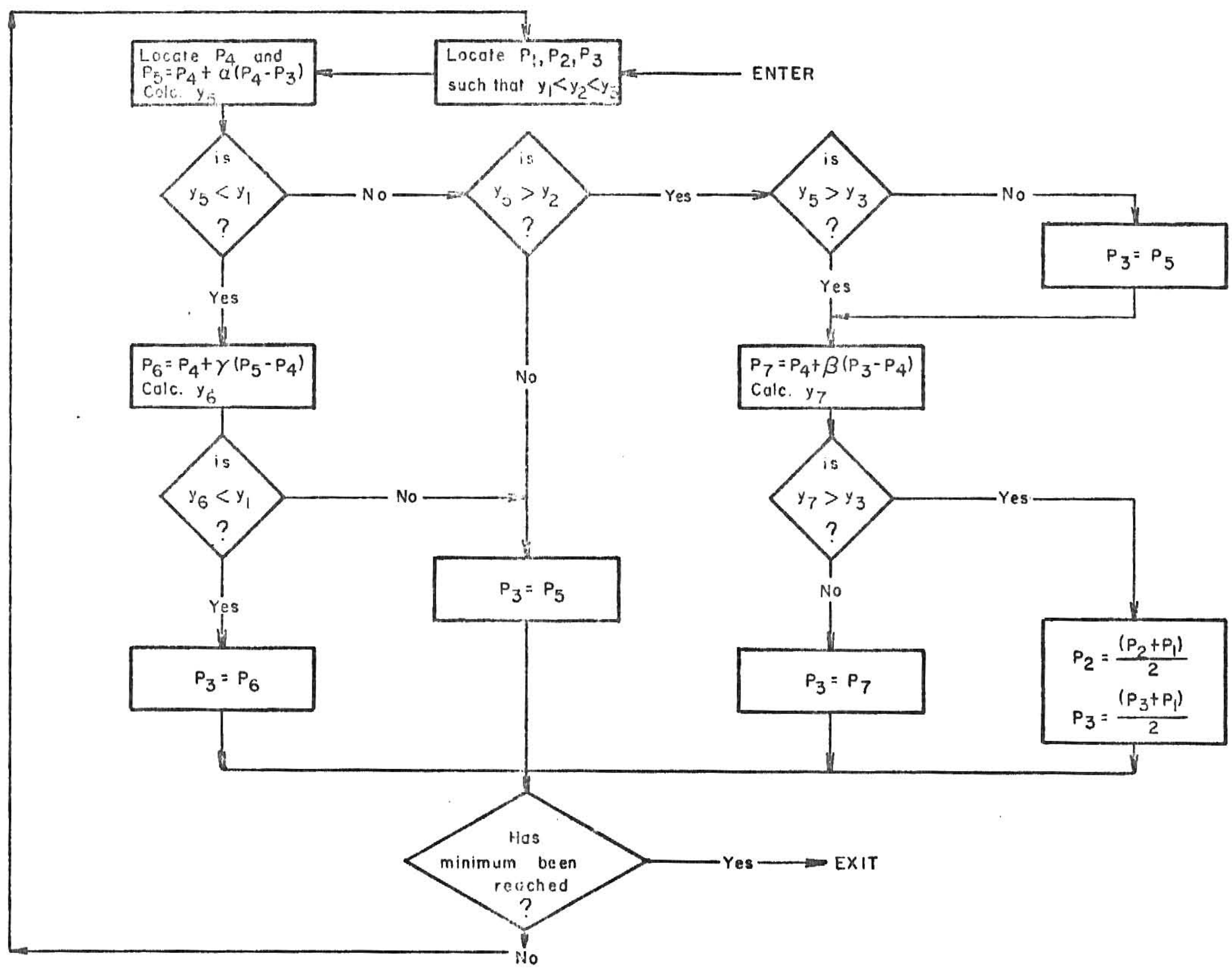

Fig. A-4.2.1 Flow diagram for the Simplex Method

APPENDIX 4.3

SYSTEM WITH NOISY INPUT AND NOISY MEASURED OUTPUT

Figure A-4.3.1 shows a diagram which represent System 3. System 3 has a noisy input and a noise-corrupted output. The input signal, y, is made up of a deterministic component, d, and a stochastic component, N_1. The output signal, Z^1, is corrupted be additive noise, N_2, producing a noise-corrupted output, Z. The parameters k_r and Z have been estimated for System 3 using Bard's method and the Simplex method. Results are presented in Tables A-4.2.1 to A-4.2.4. Table A-4.2.5 shows the value of the criterion function, S, the number of function evaluations needed to reach the optimum S, and the execution time corresponding to the sequence of data for $\sigma = 10^{-4}$ through 10^{-1}. Results obtained for System 3 are similar to results obtained for System 2 (See Tables 4.6 through 4.10).

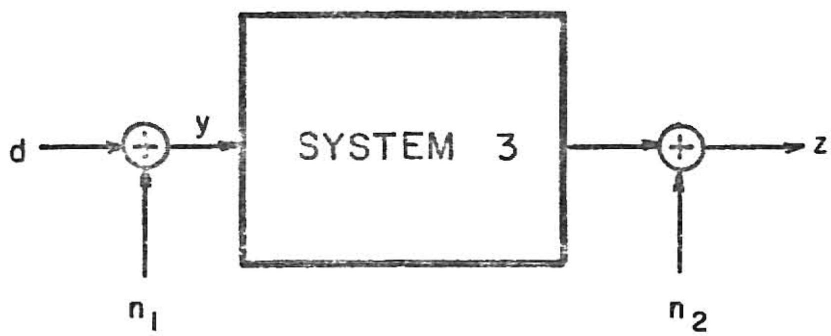

Fig. A-4.3.1 Graphical representation of System 3

Table A-2.4.1 Estimated Values of Parameter for $\sigma = 10^{-4}$

System 3

	Bard's Method		Simplex Method
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.360074	0.8140×10^{-3}	0.319692
τ	0.999763	0.2356×10^{-2}	0.113207×10^{1}

Table A-2.4.2 Estimated Values of Parameter for $\sigma = 10^{-3}$

System 3

Parameter (1)	Bard's Method: Final Estimates (2)	Bard's Method: Standard Deviation (3)	Simplex Method: Final Estimates (4)
k_r	0.372690	0.7406×10^{-2}	0.379885
τ	0.964510	0.1995×10^{-1}	0.945541

Table A-2.4.3 Estimated Values of Parameter for $\sigma = 10^{-2}$

System 3

	Bard's Method		Simplex
Parameter (1)	Final Estimates (2)	Standard Deviation (3)	Final Estimates (4)
k_r	0.285738	0.4419×10^{-1}	0.315639
τ	0.127475×10^{1}	0.2078	0.114820×10^{1}

Table A-2.4.4 Estimated Values of Parameter for $\sigma = 10^{-1}$

System 3

Parameter (1)	Bard's Method Final Estimates (2)	Bard's Method Standard Deviation (3)	Simplex Final Estimates (4)
k_r	0.781792×10^{-1}	0.2473×10^{-1}	0.281146
τ	0.545527×10^{1}	0.2128×10^{1}	0.129891×10^{1}

Table A-2.4.5 Other Estimates Used for Evaluation of the Methods

System 3

	Bard's Method			Simplex		
Standard Deviation, σ (1)	Criterion Function (2)	Function Evaluations (3)	Execution Time* (4)	Criterion Function (5)	Function Evaluations (6)	Execution Time* (7)
10^{-4}	0.3711×10^{-6}	41		0.3136×10^{-4}	32	
10^{-3}	0.2461×10^{-4}	34		0.2576×10^{-4}	33	
10^{-2}	0.1975×10^{-2}	123		0.2007×10^{-2}	37	
10^{-1}	0.1962	218	2.22 min	0.2245	37	1.14 min

*Total execution time for four values of σ

CHAPTER 5

EXPERIMENTAL SIMULATION OF STOCHASTIC STREAM RESPONSE TO THERMAL INPUTS AND APPLICATION OF SPECTRAL ANALYSIS TECHNIQUES

5.1 INTRODUCTION

The attainment of required water quality standards in streams has created a need for continuous monitoring of water quality parameters. The data obtained from these monitoring stations are complex and random in nature. One of the most effective approaches in analyzing such data to understand how various inputs such as waste treatment discharge, agricultural runoff, and meteorological events affect water quality, is the use of spectral analysis techniques. These techniques are specially designed to analyze time series data (Jenkins and Watts, 1969; Blackburn, 1970) and are effective in identifying the character of the physical phenomenon from a given time series record.

Several investigators (Wastler, 1963; Gunnerson, 1966; Thomann, 1967, 1969; Fan et al., 1970; Shastry et al., 1972) have applied these techniques to specific problems in water quality management. The work done so far pertains to calculation and interpretation of individual power spectra and cross-spectral analysis of the water quality variables.

The major difficulty in interpreting the results from spectral analysis of field data is that stream quality is constantly affected by severe chance events such as drastic changes in local weather conditions, instrument breakdown, violation of waste discharge, etc. This makes it difficult to correctly identify and interpret many of the periodicities in the power spectrum. To gain additional experience in analyzing and interpreting such complex data, it is highly desirable to conduct controlled experiments and examine the effects of these random events on the spectral estimates. Such an effort will enhance our capability to judiciously analyze field data and suggest improvements in the data analysis procedures.

In this study, an experimental simulation of stream response to monitored inputs was carried out. The purpose was two-fold: first, to test the general validity of spectral analysis techniques in analyzing noisy water quality data, and second, to see how accurately the known periodicities in the input spectrum could be recovered from the measured output response in the presence of noisy disturbances. Temperature was chosen as the water quality parameter. The data were obtained by superimposing cyclic and non-cyclic signals (monitored discharges) of temperature (using steam as signal) on the inherently noisy signals of the stream. The response to these monitored discharges was analyzed by spectral analysis techniques. The applicability of some of these results to water quality monitoring is discussed in this chapter.

5.2 EXPERIMENTAL

An experimental stream channel, 30 inches in length, 12 inches in width, and of variable depth, was used in this investigation. A schematic diagram of the experimental set-up is shown in Fig. 5.1. Cold water was continuously fed to the system, and the flow rate was continuously monitored with a ratameter. Monitored cyclic and non-cyclic thermal discharges were also fed at the inlet and the response.

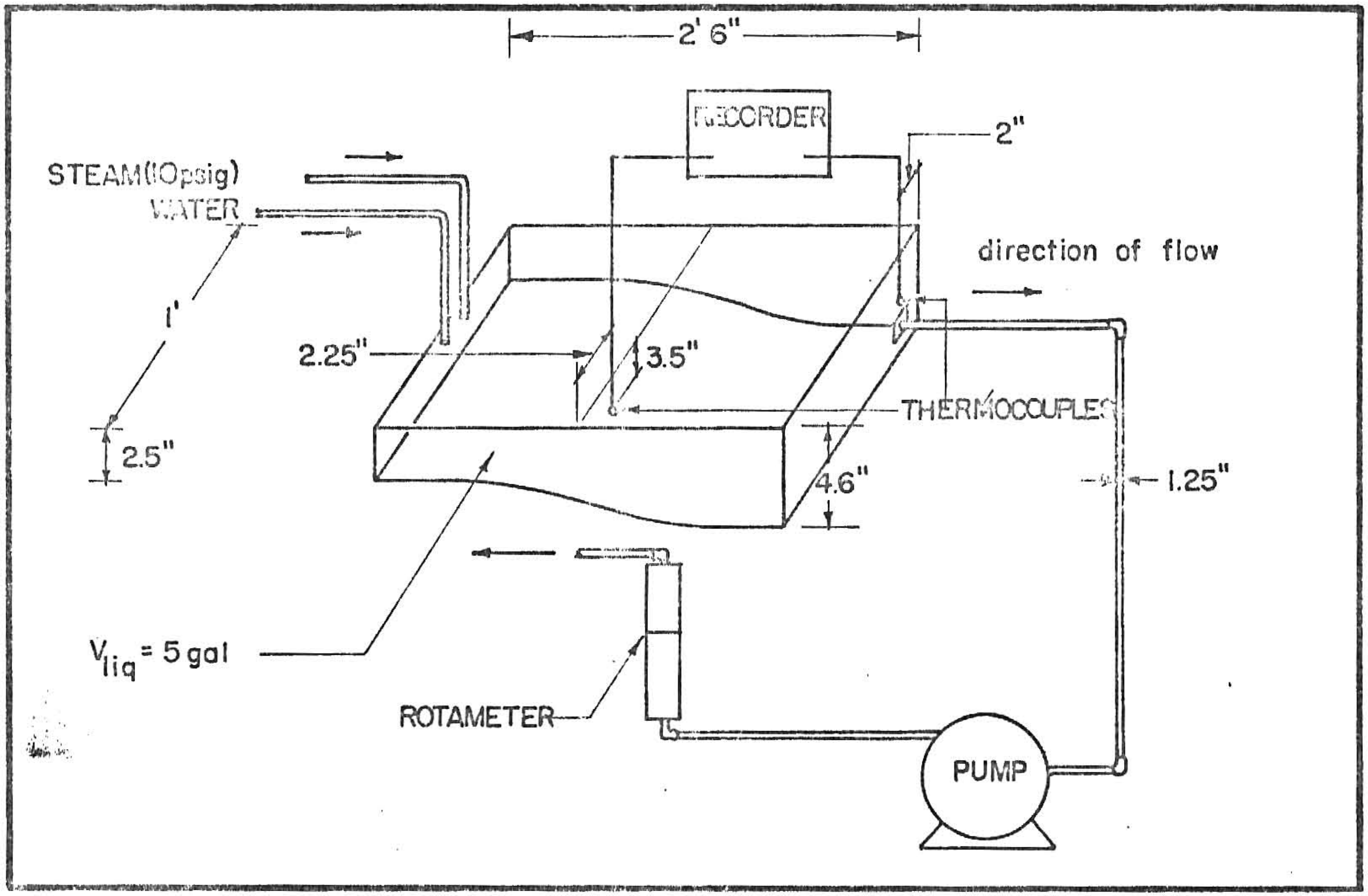

Fig.5.1. Experimental Set-up

to these discharges was measured at two different points along the stream. Steam was used as the thermal discharge. Two thermocouples, one for each position of measurement, were used to record continuously the temperature variations. The measurement points are referred to as 'middle temperature' and 'outlet temperature' locations. The 'middle temperature' thermocouple was located near the wall of the experimental channel as shown in Fig. 5.1. The 'outlet temperature' position was located at the exit.

Four experiments were conducted using two different flow rates and two types of thermal discharge. A continuous thermal input was employed for Experiments 1 and 3, while for Experiments 2 and 4, the steam flow rate was cycled with an 'on-off' twenty second period as shown in Fig. 5.2. Table 5.1 gives the flow rates and type of thermal discharge employed in each experiment.

Middle and outlet temperature data were continuously recorded onto strip charts for a duration of about 15 minutes for each of the experiments. A temperature of $68^{\circ}F$ was used as the base temperature in analyzing the data. The range of deviations from the base temperature was about $1^{\circ}F$ and the deviations were digitized at one and two second intervals for the experimental conditions outlined in Table 5.1.

A modified version of the BMD02T computer program (University of California, Health Sciences Computing Facility, 1967) was used to evaluate the spectral estimates on an IBM system 360/50 digital computer. A summary of the mathematical expressions for each estimate can be found in Table 5.2 (Blackman and Tukey, 1958; Box and Jenkins, 1970; Shastry et al., 1972).

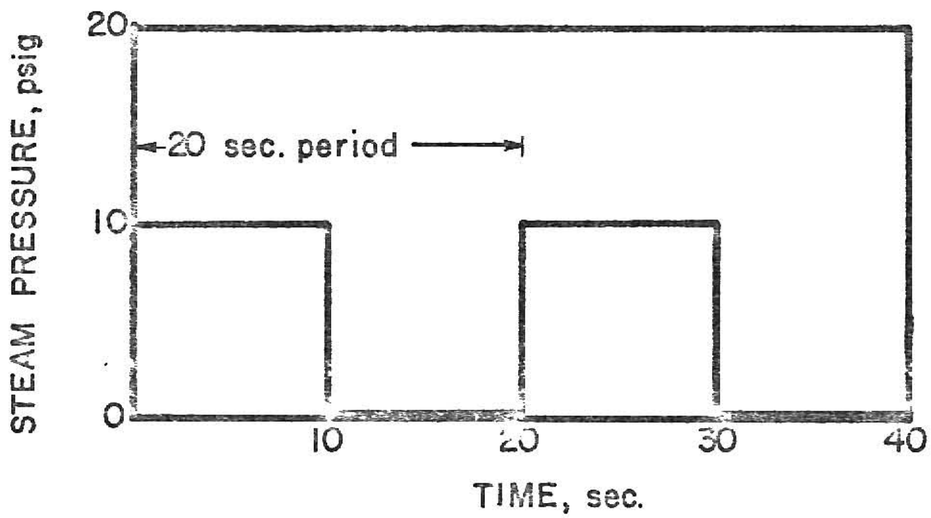

Fig.5.2. The periodic on-off steam flow rate used in Experiments 2 and 4.

Table 1. Experimental Conditions

Experiment No.	Flow rate (gal/min)	Thermal discharge	Number of data points digitized	Time interval Δt (sec)	Variance of the raw records	
					Middle temperature	Outlet temperature
1	5	cont.	380	1	0.0122	0.0325
1	5	cont.	380	2	0.0097	0.0178
2 (Subset 1)	5	cyclic	380	1	0.0046	0.0061
2 (Subset 2)	5	cyclic	380	1	0.0168	0.1021
2 (Subsets 1 & 2)	5	cyclic	760	1	0.0108	0.0597
3	1	cont.	380	1	0.0211	0.1617
4	1	cyclic	380	1	0.0093	0.0372

Table 5.2 Information to be Obtained During Spectral Analysis

Function	Formula	Remarks
Autocorrelation	$R_{xx}(\tau) = \frac{1}{T} \int_{-\infty}^{\infty} X(t)\, X(t+\tau)dt$ $\lim_{T\to\infty} \frac{1}{T} \int_{0}^{T-\tau} X(t)\, X(t+\tau)\, dt$	1. autocorrelation means correlation with itself 2. at zero lag autocorrelation equals the variance 3. it is symmetrical about zero lag 4. can be used for elimination of random and systematic errors
Spectral estimate	$S_{xx}(w) = \frac{1}{2\Pi} \int_{-\infty}^{\infty} R_{xx}(\tau) e^{-iw\tau} d\tau$	1. spectral estimate identifies periodicities in the record 2. provides correlation in the frequency domain
Crosscorrelation	$R_{xy}(\tau) = \frac{1}{T} \int_{-\infty}^{\infty} X(t)\, Y(t+\tau)\, dt$	1. gives a correlation between two time series 2. not symmetrical about zero lag 3. can be used for elimination of errors resulting from phase differences

Table 5.2 Continued

Function	Formula	Remarks
Cross spectrum	$S_{xy}(\tau) = \frac{1}{\Pi} \int_{-\infty}^{\infty} R_{xy}(\tau) e^{-iw\tau} d\tau$	1. correlation between two series in frequency domain 2. useful in computing transfer function and coherence square
Transfer function	$\lvert H(w) \rvert = \left(\frac{SP_{yy}(w)}{SP_{xx}(w)}\right)^{1/2}$ $H(w) = \frac{SP_{xy}}{SP_{xx}}$	1. relates output to the input in the frequency domain 2. can be used for developing mathematical model 3. calculation of cross spectra is necessary if any information about the phase angel is desired
Coherence square	$\gamma_{xy}^{2} = \frac{SC_{xy}^{2} + SQ_{xy}^{2}}{SP_{xx}\, SP_{yy}}$	1. is a measure of the linearity of the system 2. investigates correlation is small range of frequencies

5.3 RESULTS AND DISCUSSION

The effect of sampling interval on the results of spectral analysis was investigated by digitizing the continuous record at both one second and two second intervals. This effect is illustrated in Figs. 5.3 and 5.4 using outlet temperature data for Experiment 1 (Fig. 5.3) and middle temperature data for Experiment 2 (Fig. 5.4). The autocorrelation and power spectrum results presented in Figs. 5.3 and 5.4 indicate that either of the sampling intervals used to digitate the data in Experiments 1 and 2 provides esentially the same information. For both sampling intervals, the autocorrelation function decreases toward zero at approximately the same rate and the periodicities due to the periodic thermal discharge are similar. The significant peak at 0.05 cycle/sec which appears in the power spectrum for Fig. 5.4 is predicted equally well by each of the sampling intervals. A sampling interval of one second was used to digitize other records.

Visual examination of the record obtained from Experiment 2 indicated that the oscillations about the average temperature were smaller in the first half of the record than in the second half of the record. The total record was divided into two subsets, and the stationarity of each subset was examined separately. The first subset of 380 data points was obtained from the first half of the record (from a nomical zero time of recording up to 380 seconds). The second subset of 380 data points was obtained from the second half of the record (from 510 seconds up to 890 seconds). Two sets of 760 data points were made by combining the first and second subsets for each of the two thermocouple locations.

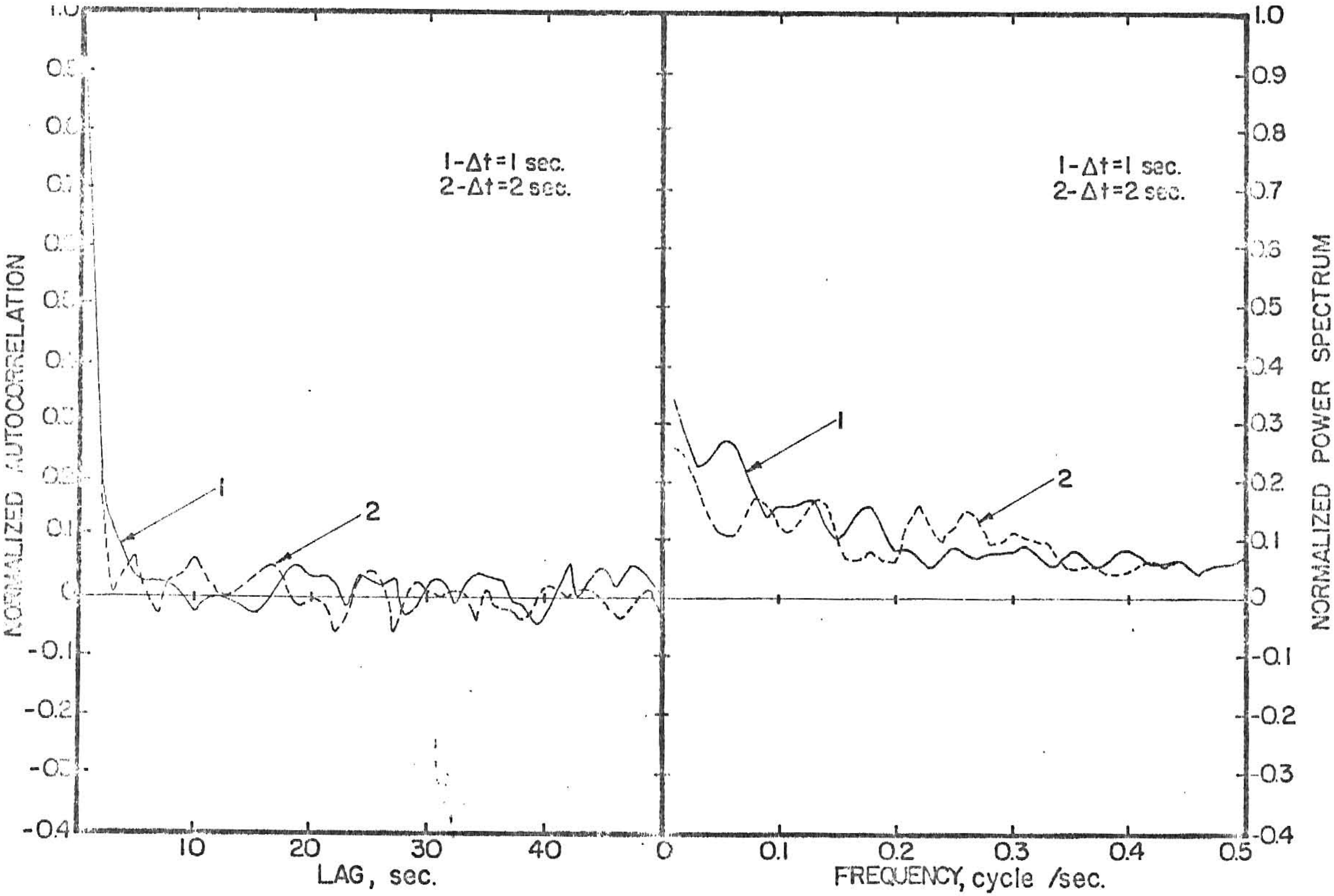

Fig.5.3. Effect of sampling interval on autocorrelation and power spectrum for Experiment I (continuous steam input, outlet temperature).

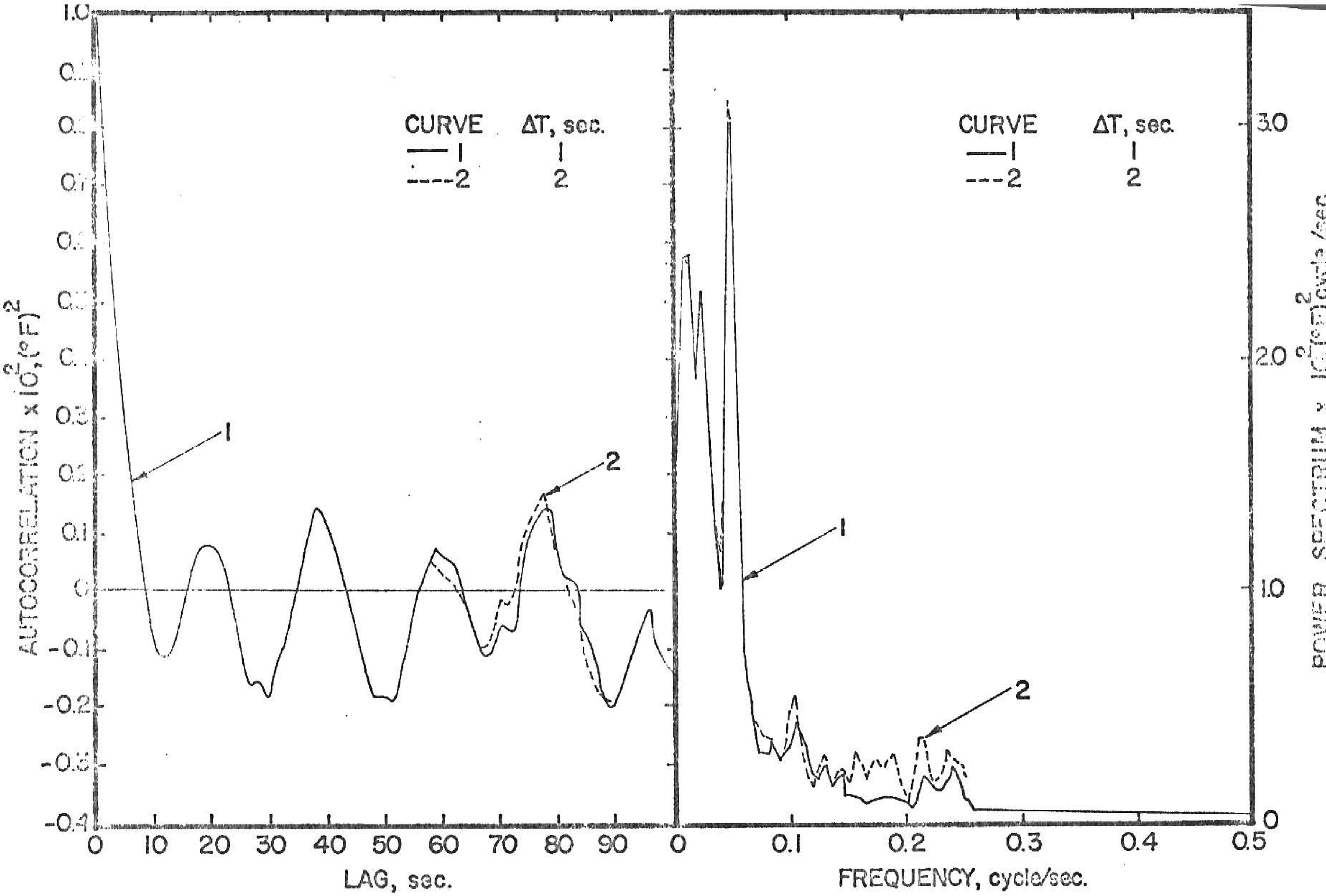

Fig.5.4. Effect of sampling interval on autocorrelation and power spectrum for Experiment 2 (periodic steam input, middle temperature).

The normalized autocorrelation and power spectrum for each set of data are shown in Figs. 5.5 and 5.6, respectively, for the middle temperature record, and in Figs. 5.7 and 5.8 for the outlet temperature record. In Figs. 5.5 through 5.8, Curve 1 represents the first subset, Curve 2 the second subset, and Curve 3 the set of data made up of subsets 1 and 2.

An inspection of Fig. 5.5 reveals that the periodicities in the autocorrelation function are similar for the second subset (Curve 2) and the set made up of subset 1 and subset 2 (Curve 3). The first subset (Curve 1) shows more periodicities than the other two records for the same lag. The power spectrum for the middle temperature record (see Fig. 5.6) also shows this similarity between Curves 2 and 3 in that the peak corresponding to the periodic thermal discharge (20 seconds period) at 0.05 cycles/sec is distinct in both curves. Curve 1 does not predict this peak distinctly.

At the outlet, the similarity between subset 2 and the set made up of subsets 1 and 2 still persists. The normalized autocorrelation function (see Fig. 5.7) is always positive for all lags for subset 2 (Curve 2) and the set made up of subsets 1 and 2 (Curve 3), whereas for subset 1 (Curve 1), the autocorrelation function drops to zero near a lag of 10 secs and then oscillates about zero. The power spectrum estimates in Fig. 5.8 show that only the first subset predicts the peak at 0.05 cycles/sec corresponding to the periodic thermal discharge which is the reverse of the result obtained at the middle temperature location.

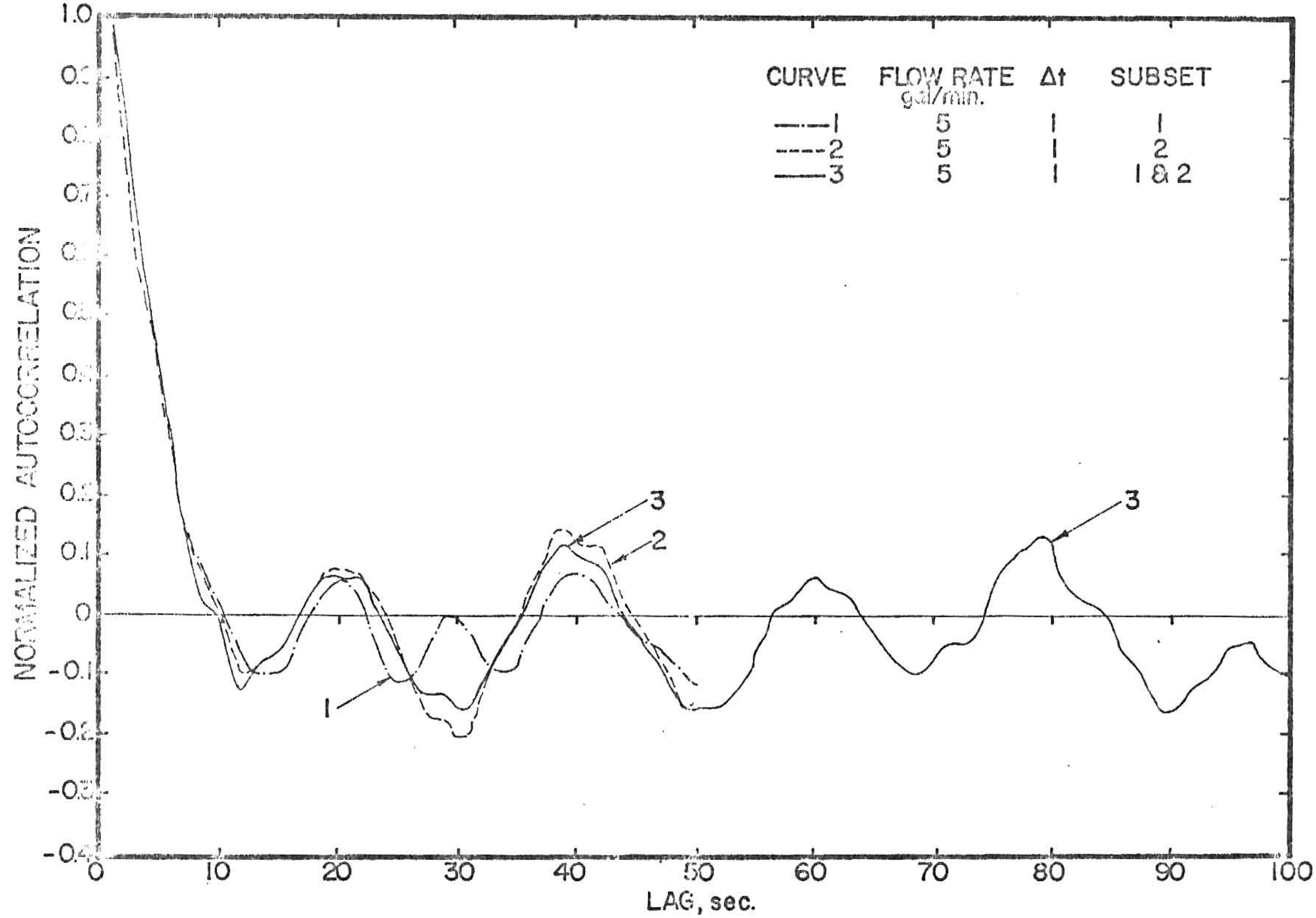

Fig.5.5. Effect of total time period of sampling on normalized autocorrelations for Experiment 2 (periodic steam input, middle temperature).

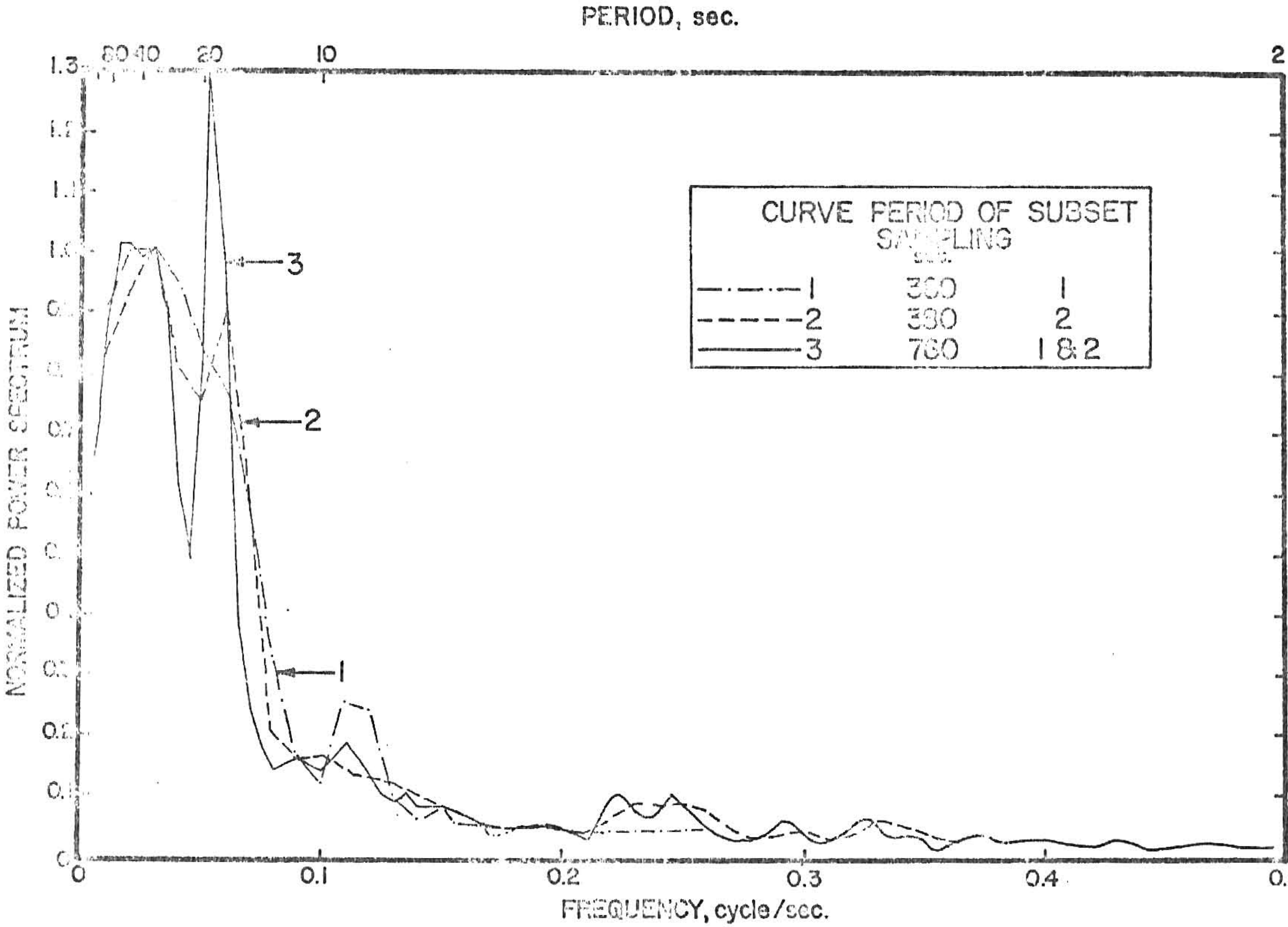

Fig.5.6. Effect of total time period of sampling on normalized power spectrum for Experiment 2 (periodic steam input, middle temperature).

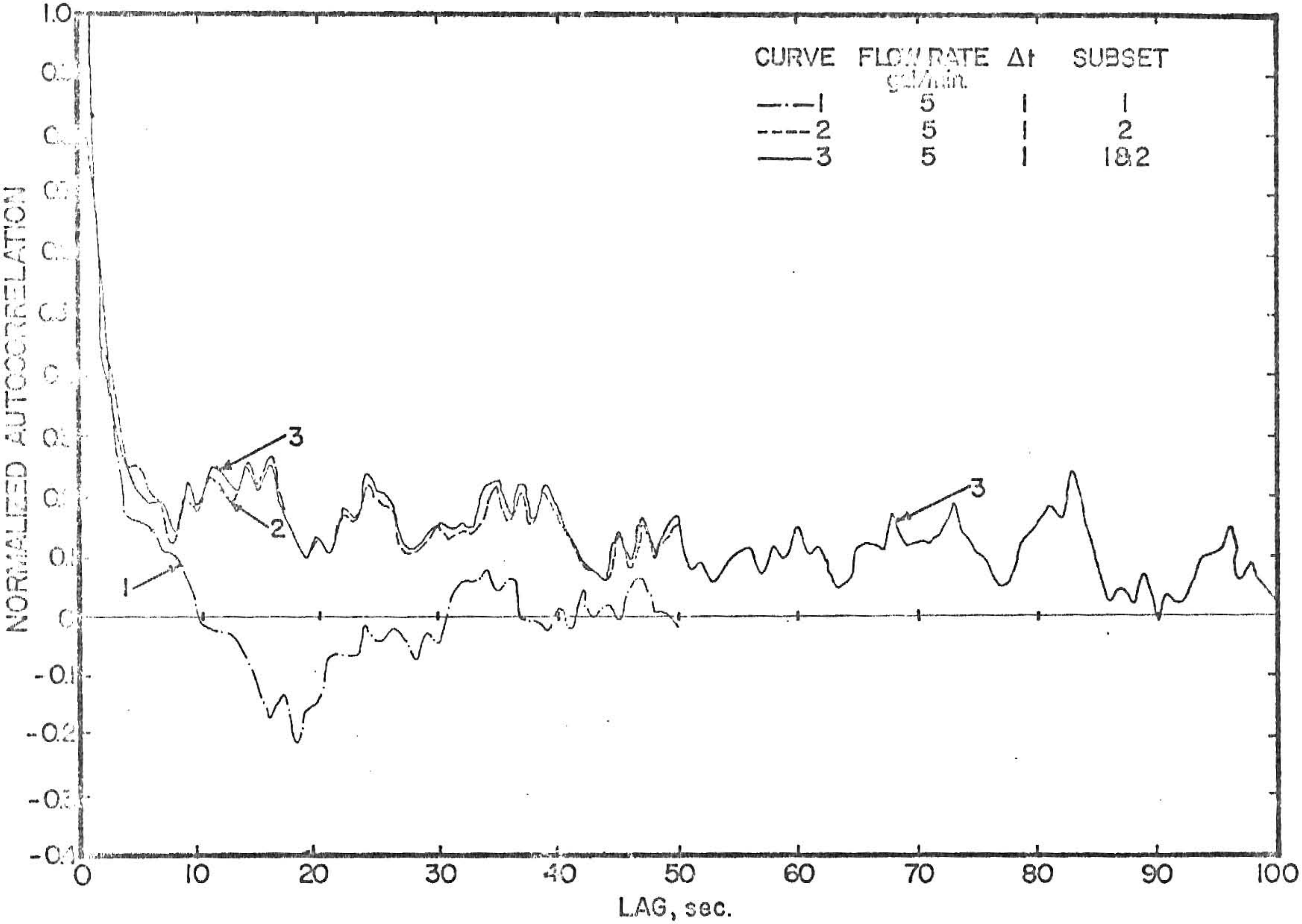

Fig.5.7. Effect of total time period of sampling on normalized autocorrelation for Experiment 2 (periodic input, outlet temperature).

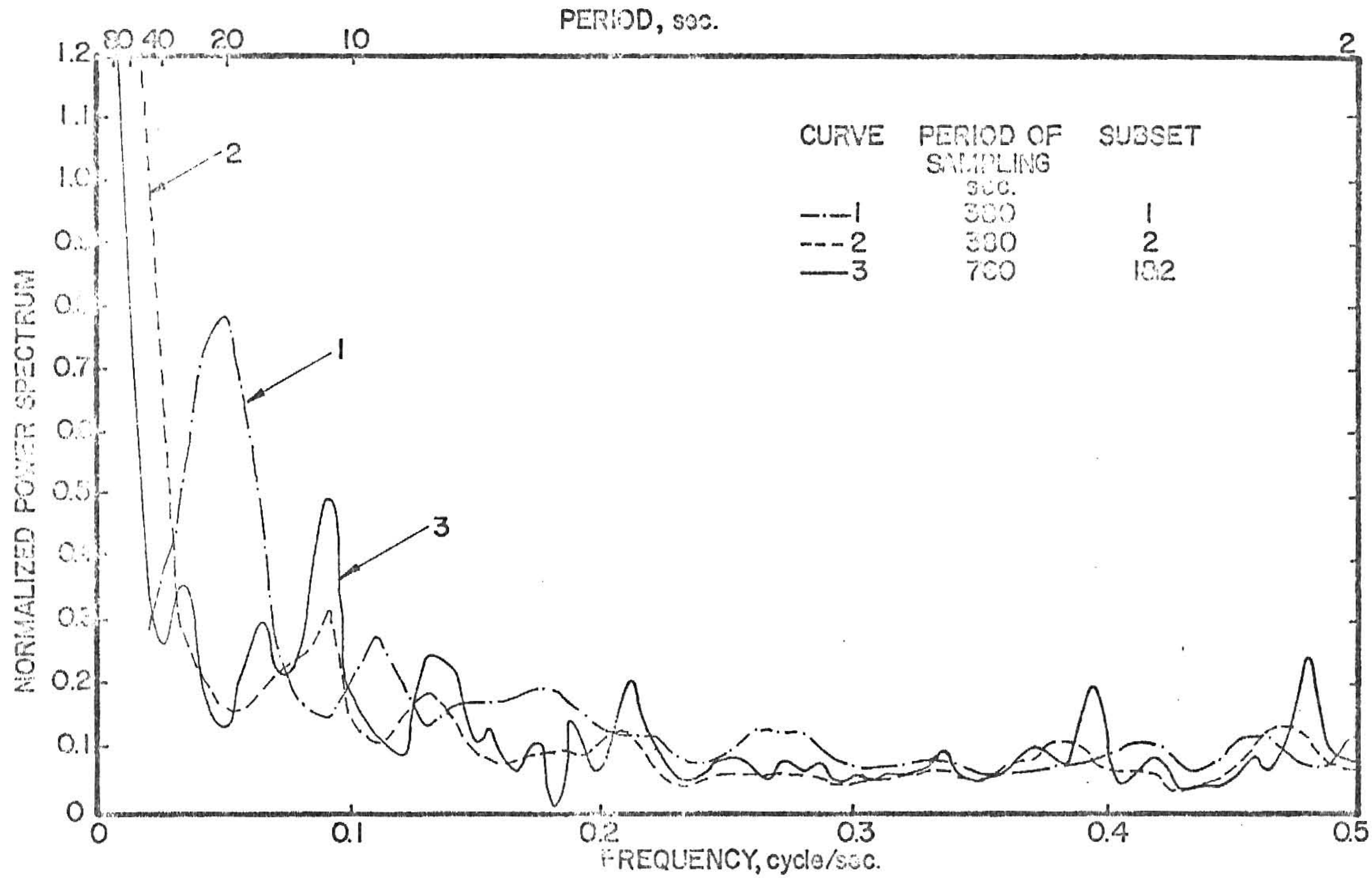

Fig.5.8. Effect of total time period of sampling on normalized power spectrum for Experiment 2 (Periodic steam input, outlet temperature).

The similarity in Curves 2 and 3 at both locations is probably due to the fact that the fluctuations about the average temperature were greater in the second half of the record that in the first half. As a result, the entire record (first and second half put together) is dominated by the second half of the record because of the larger variations there. In order to better understand these results a check for stationarity of the individual records was made at both locations.

The individual sets of data obtained in Experiment 2 at both locations were analyzed for staionarity by performing the non-parametric run test. A run is defined as a succession of identical observations which are followed and preceded by different observations or no observation at all. The number of runs of data values above or below the median value of the series is the basis for a stationarity test. The test is fairly simple, and the procedure is outlined in Bendat and Piersol (1971).

Based on the results of the run test at an α level of 0.05, it was concluded that subset 1, subset 2 and the set made up of subsets 1 and 2 at the middle temperature location were stationary. For the outlet temperature record, subset 1 and subset 2 were stationary but the set made up of subsets 1 and 2 was non-stationary. The test for stationarity was also applied to the data obtained from Experiments 1, 3 and 4, and they were all found to be stationary at an α level of 0.05.

Continuous thermal discharge

Figures 5.9 - 5.13 show the results of spectral analysis for Experiments 1 and 3 in which steam and water are fed continuously at the inlet.

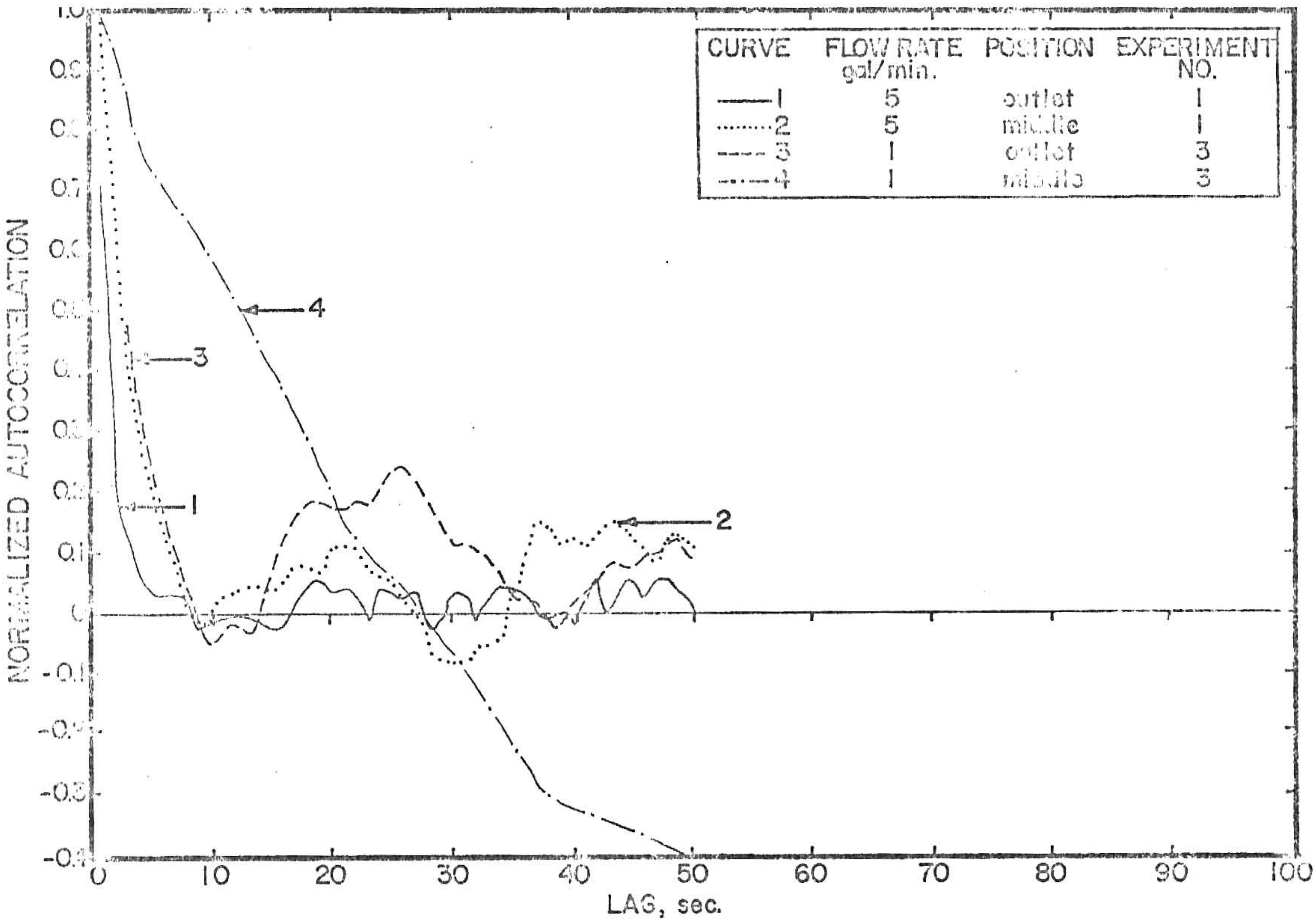

Fig.5.9. Effect of measurement position and flow rate on autocorrelation results for continuous steam input.

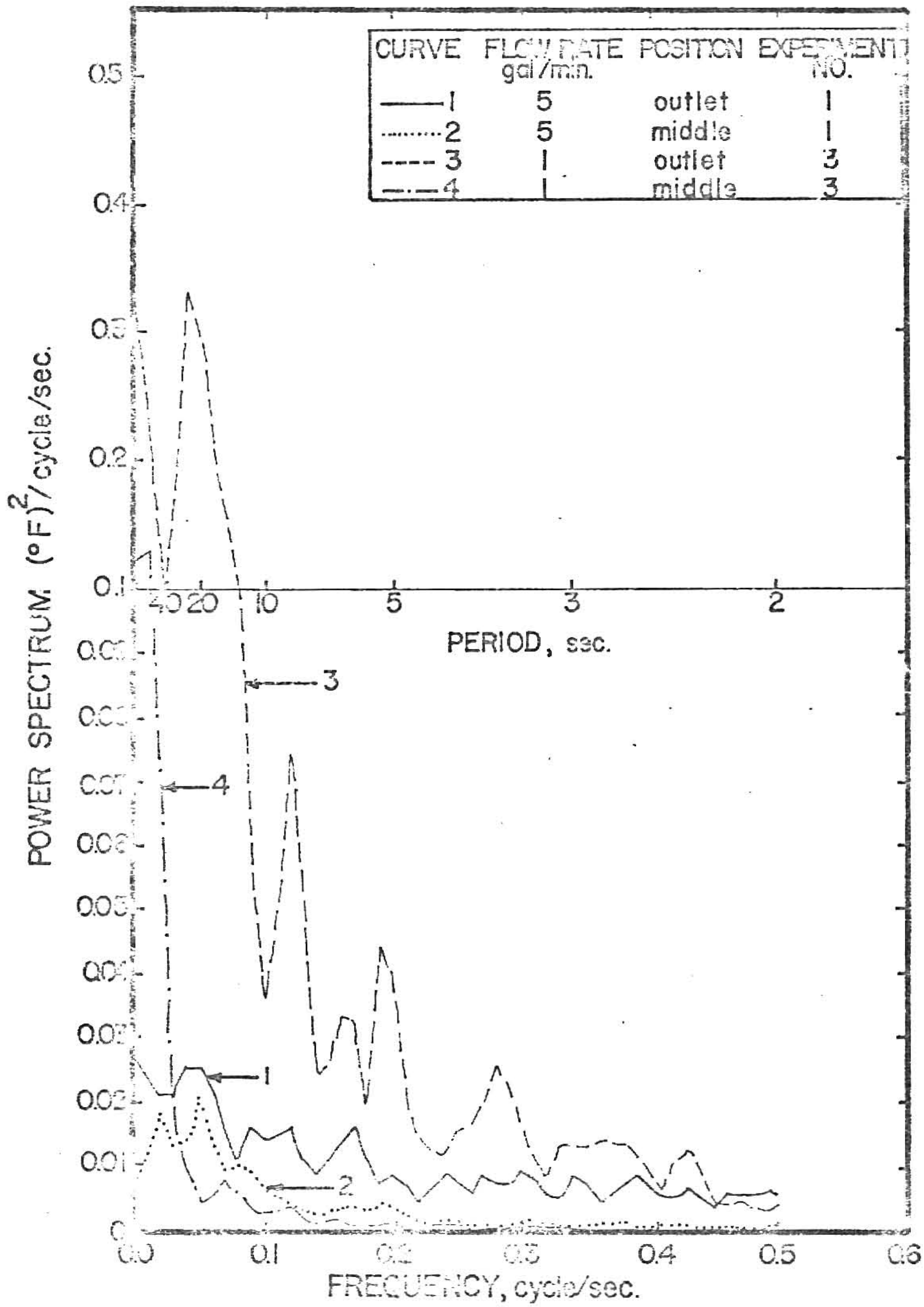

Fig.5.10. Effect of flow rate and measurement position on spectral estimates (continuous steam input).

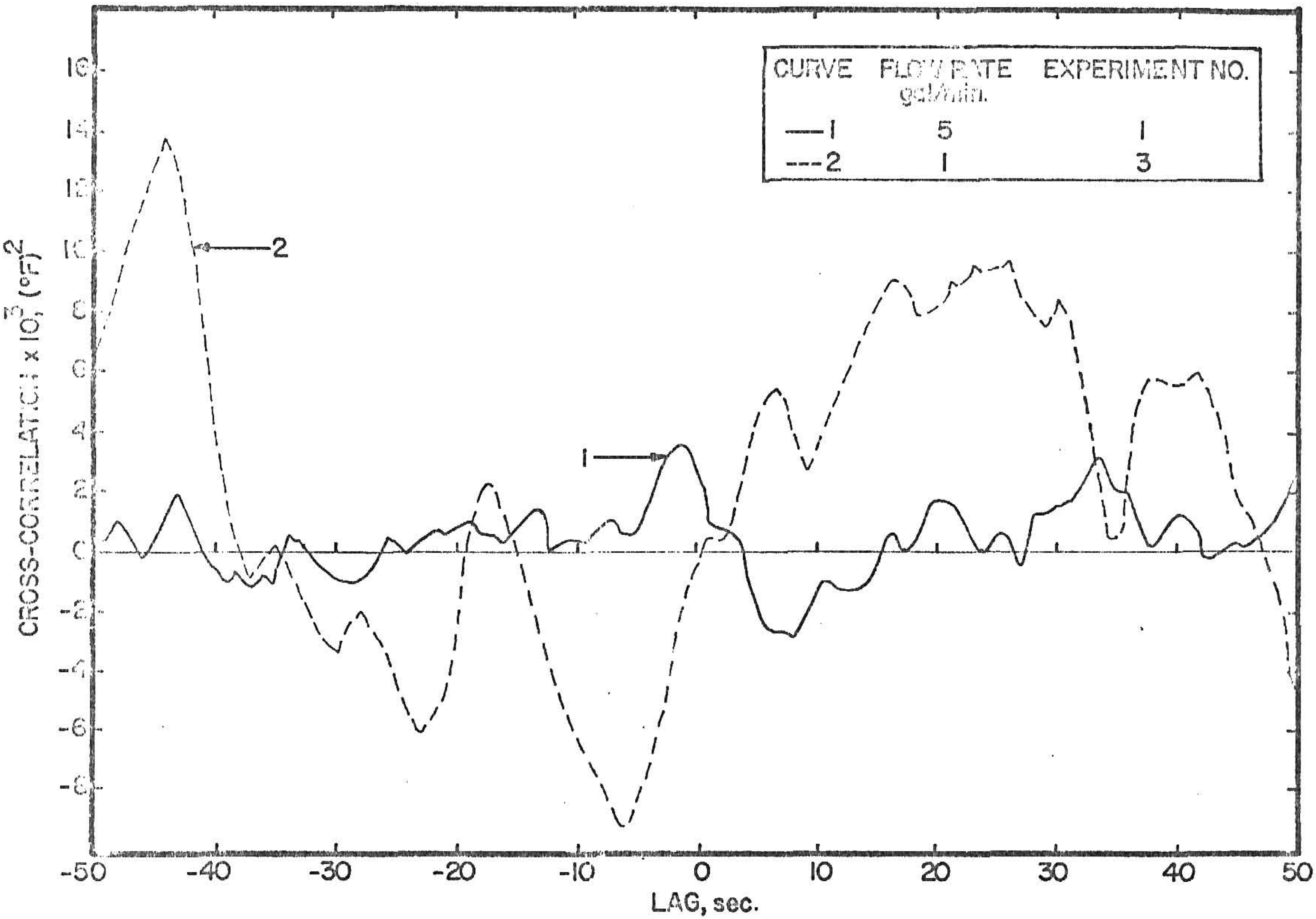

Fig.5.11. Effect of flow rate on cross-correlations between middle and outlet temperatures (continuous steam input).

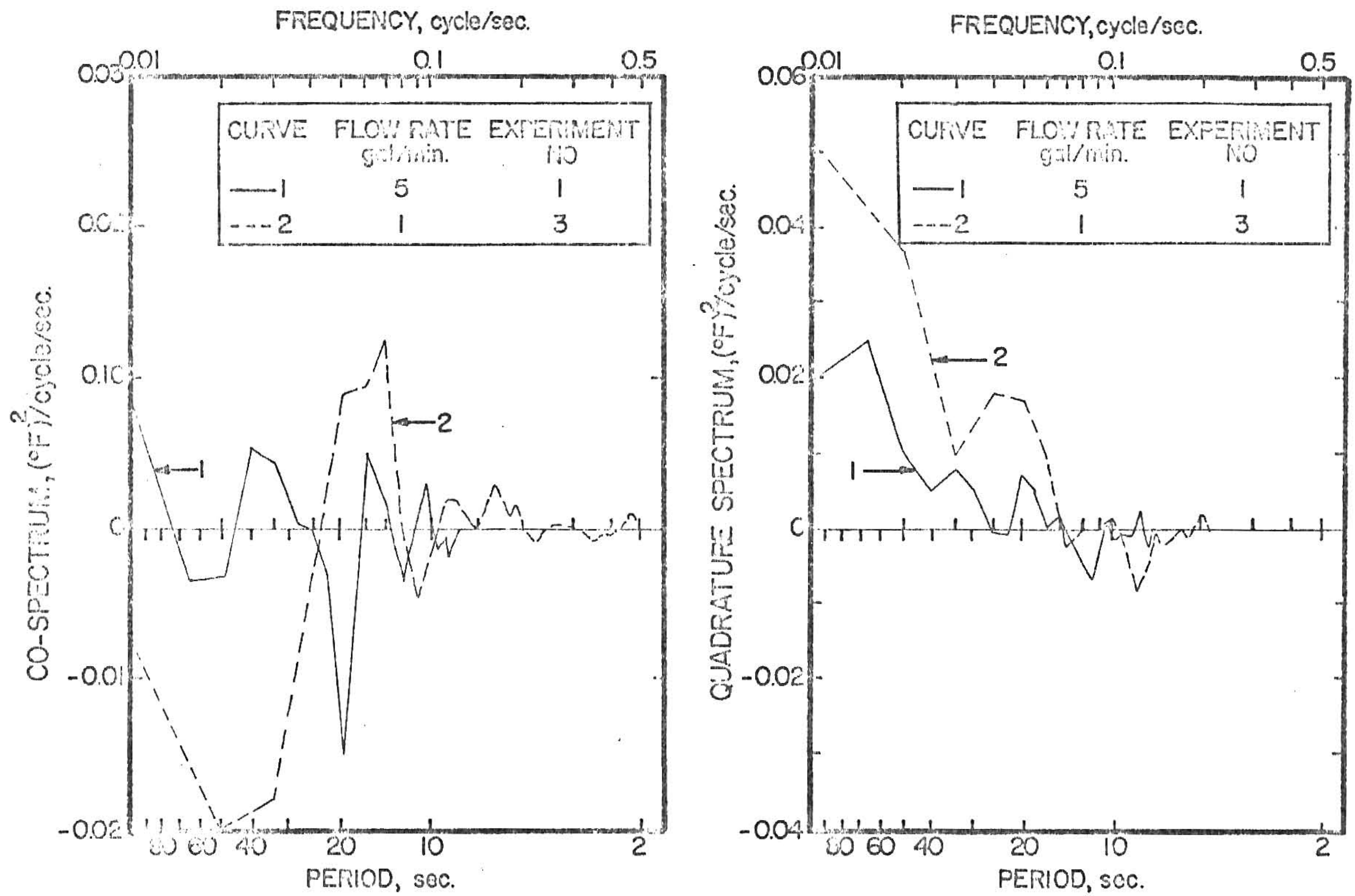

Fig.5.12. Effect of flow rate on the co-spectrum and quadrature spectrum for continuous steam input.

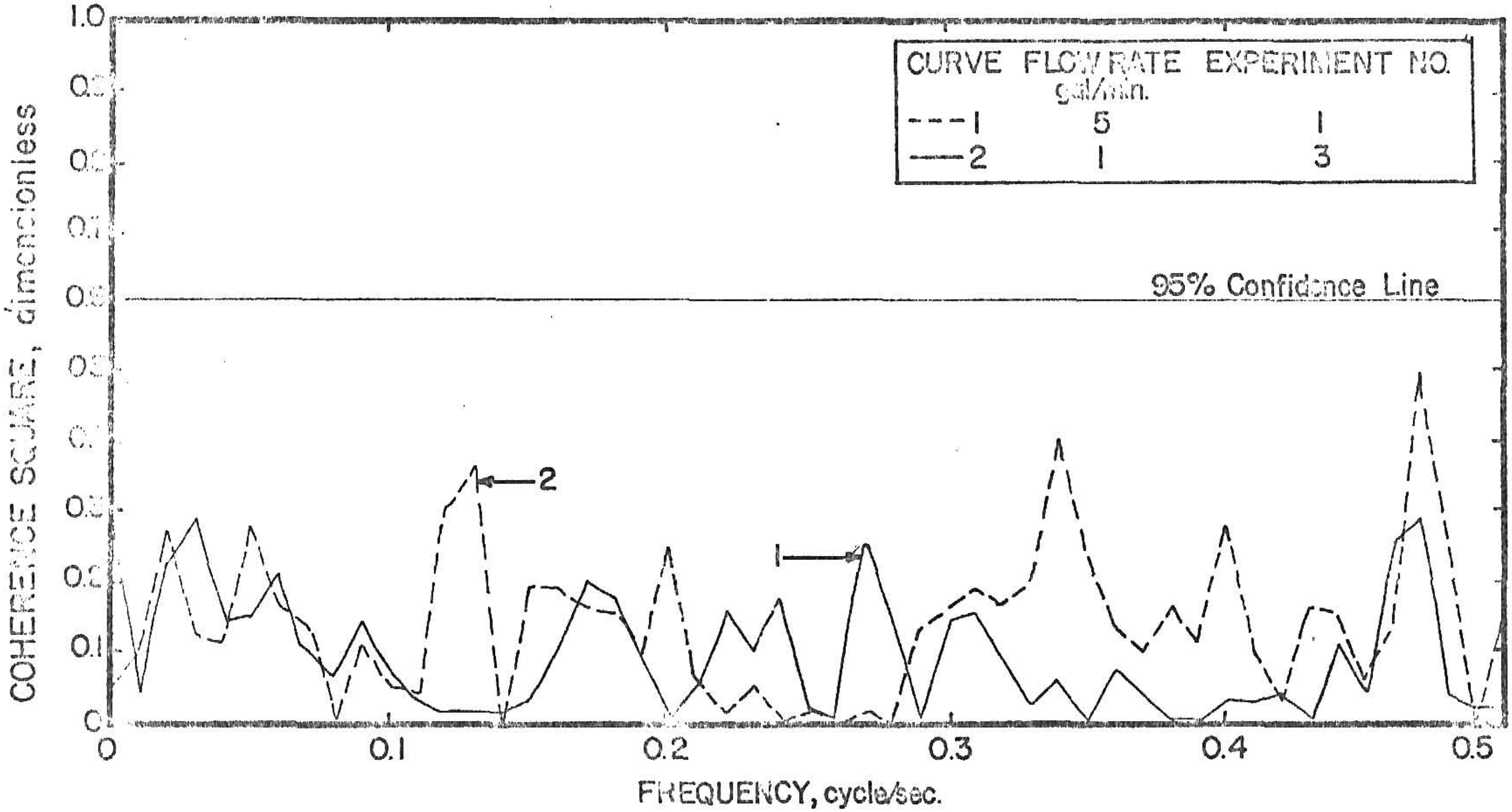

Fig.5.13. Effect of flow rate on coherence between middle and outlet temperatures for continuous steam input.

The effect of position of measurement and flow rate on the autocorrelation results can be observed in Fig. 5.9. Curves 1 and 2 represent the autocorrelation results for the temperature data obtained at the higher flow rate (5 gal/min). By comparing these results with the results shown in Curves 3 and 4, respectively, for the low flow rate data (1 gal/min), the autocorrelation function diminishes much more rapidly to zero and is less persistent for the high flow rate record than for the low flow rate record. This may be attributed to the turbulent motion of the fluid which is greatly enhanced by rapid mixing of the streamlines, sudden change in cross-sectional area (contraction), interaction of the fluid elements with the solid walls of the channel, and subsequent rapid fluctuations in the temperature record. These effects make the successive temperature values become uncorrelated after a short lag. As far as the position of measurement is concerned, autocorrelation results of the outlet temperature records (Curves 1 and 3) indicate very little correlation in the successive temperature values as compared to the middle temperature records (see Curves 2 and 4). This is expected, since there is greater attenuation of the signal (temperature response) at the outlet. In addition, turbulent effects are predominant at the outlet as mentioned above.

The power spectra for Experiments 1 and 3 are shown in Fig. 5.10. Since a continuous thermal input is employed in these experiments, no obvious spectra that can be attributed to controlled thermal discharge transients can be observed. The results show considerably larger values of the power spectra for Curve 3 (outlet temperature, flow rate 1 gal/min) than for Curves 1 and 2. These larger values could result from variations in the circulation pattern within the vessel or from other variations which repeated themselves sufficiently to appear on the power spectrum.

The cross-correlations between the middle temperature and the outlet temperature are shown in Fig. 5.11 for Experiments 1 and 3. For Experiment 1 (flow rate = 5 gal/min), the magnitude of the cross-correlation is small, and the curve appears to vary rapidly and randomly with lag. At the lower flow rate (1 gal.min), the magnitude of the cross-correlation is greater, and there are fewer fluctuations. The cross-spectral estimates in Fig. 5.12 can be used to judge the extent of cross-correlation between temperatures at these two locations. For Experiment 3 the co-spectrum is negative for periods greater than 25 seconds. This implies that the value of the corresponding cross-correlation should also be negative for lags greater than 25 seconds (Panofsky and Brier, 1968). Since the cross-correlation results obtained here are not consistent with the co-spectrum results, one can conclude that any cross-correlation between these two temperatures which may exist is hidden by random fluctuations.

Examination of the coherence between middle and outlet temperatures also indicates that noise levels were very high in Experiments 1 and 3. The confidence limits for the coherence function were estimated assuming that the middle and outlet temperature records have a bivariate normal distribution (Goodman, 1957). Tables which give these limits have been presented by Granger and Hatanaka (1964). The coherence function with the 95% significance level corresponding to 7.6 degrees of freedom is presented in Fig. 5.13. Based on these results one can conclude that any correlations which exist between middle and outlet temperature records are not statistically significant at the 95% confidence level.

The amplitude of the transfer function between the middle and outlet temperatures was computed. It appeared to be independent of frequency.

Periodic thermal discharge

In Experiments 2 and 4 the thermal discharge was an on-off cycle as shown in Fig. 5.2. This type of input was selected in order to investigate the extent to which such a periodic input can be observed at downstream measuring stations. Figures 5.14 - 5.17 present the autocorrelations, power spectra, cross-correlations, and coherence, respectively, for Experiments 2 and 4.

In Fig. 5.14 the effect of the periodic input on the autocorrelation is visually apparent (see Curve 2) for the middle temperature for Experiment 2 (flow rate = 5 gal/min). The peaks corresponding to the periodic thermal discharge (20 second period) are not distinct in Curves 1 and 3. These results represent the conditions at the outlet; the noise levels are high at this position of measurement due to turbulence and other end effects previously mentioned. As a results, the periodicities corresponding to the thermal input are masked by the random fluctuations and are difficult to identify in the autocorrelation function. Figure 5.15 shows the power spectra for Experiments 2 and 4. Because of the periodic thermal discharge, there should be an observable peak at 0.05 cycles/sec (20 second period). A peak near this frequency is visible for each of these four records. For Experiment 2 the middle temperature has a definite peak at the 0.05 cycles/sec frequency (see also Figs. 5.4 and 5.6). At a flow rate of 5 gal/min, the effects of the periodic thermal input are definitely observable in both

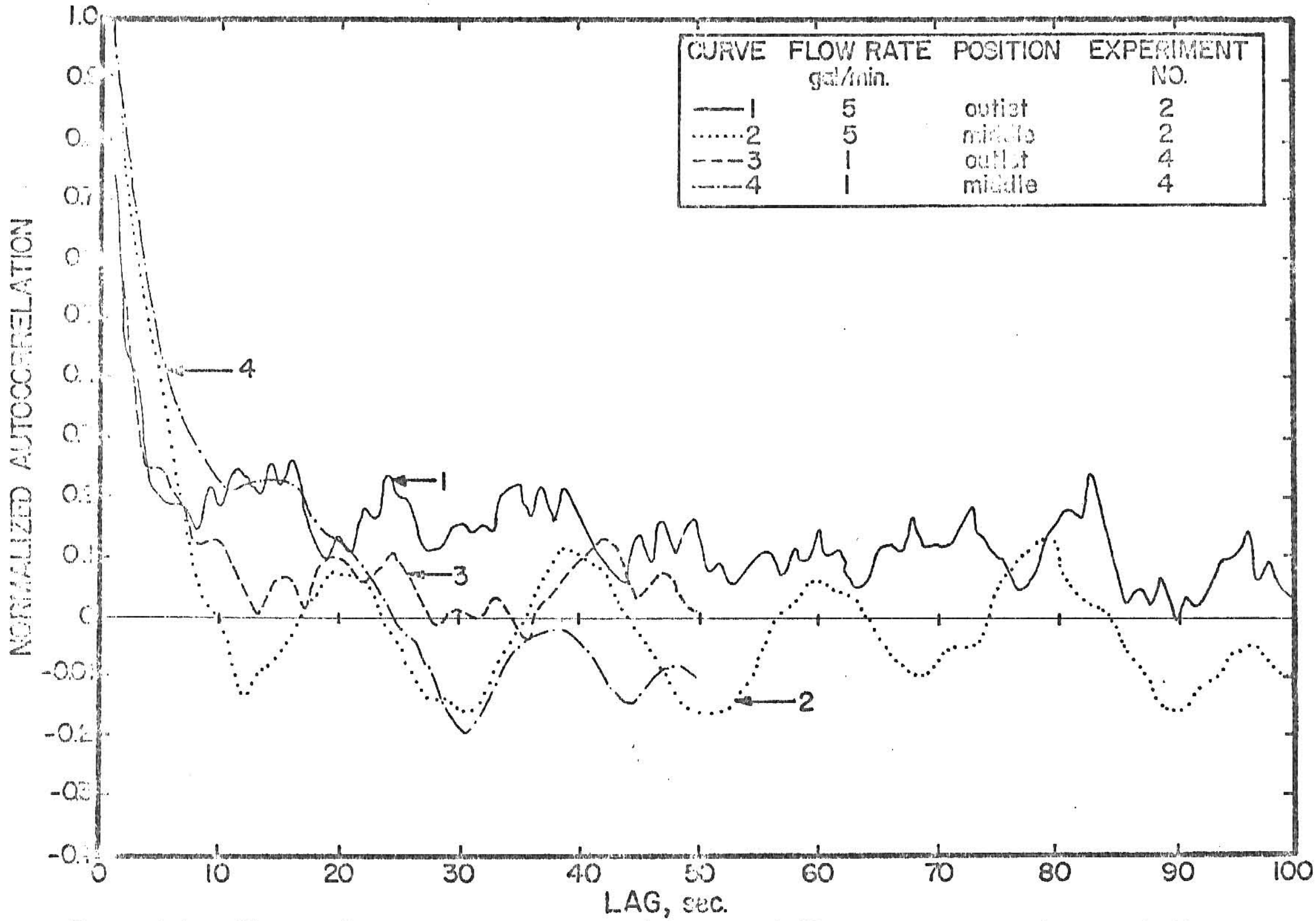

Fig. 5.14. Effect of measurement position and flow rate on autocorrelation results for periodic steam input.

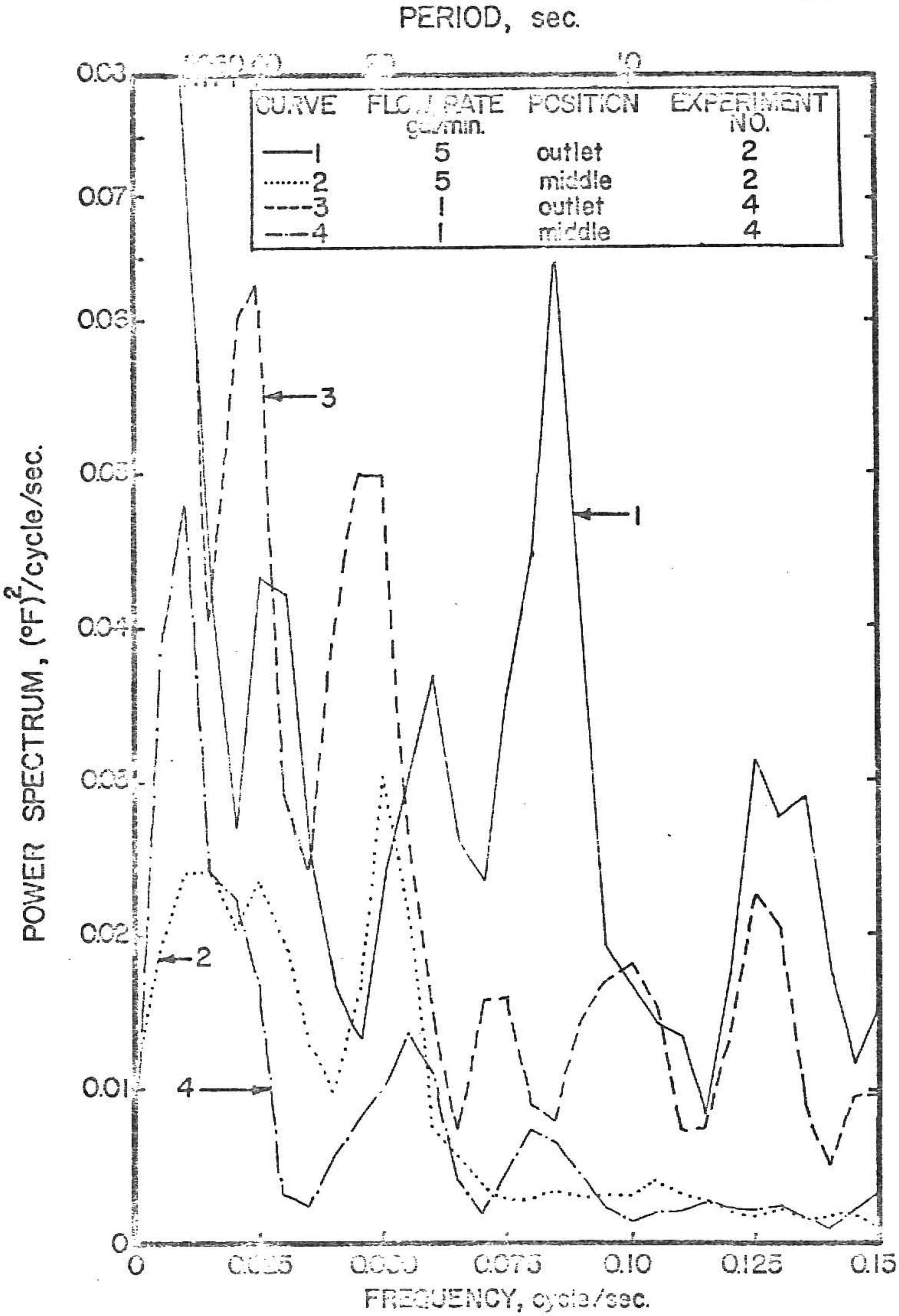

Fig.5.15. Effect of flow rate and measurement position on spectral estimates for periodic steam input.

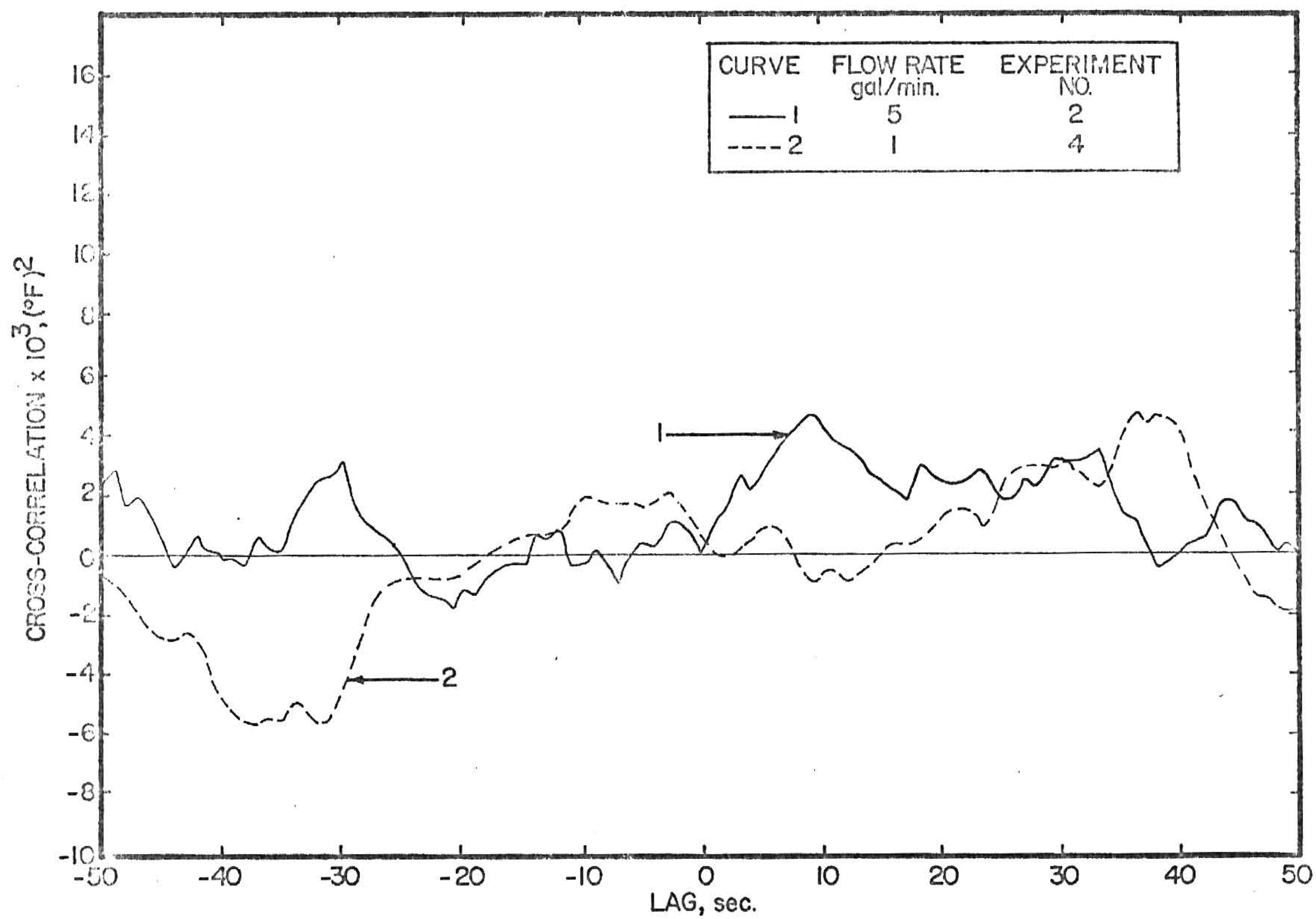

Fig.5.16. Effect of flow rate on cross-correlation between middle and outlet temperatures for periodic steam input.

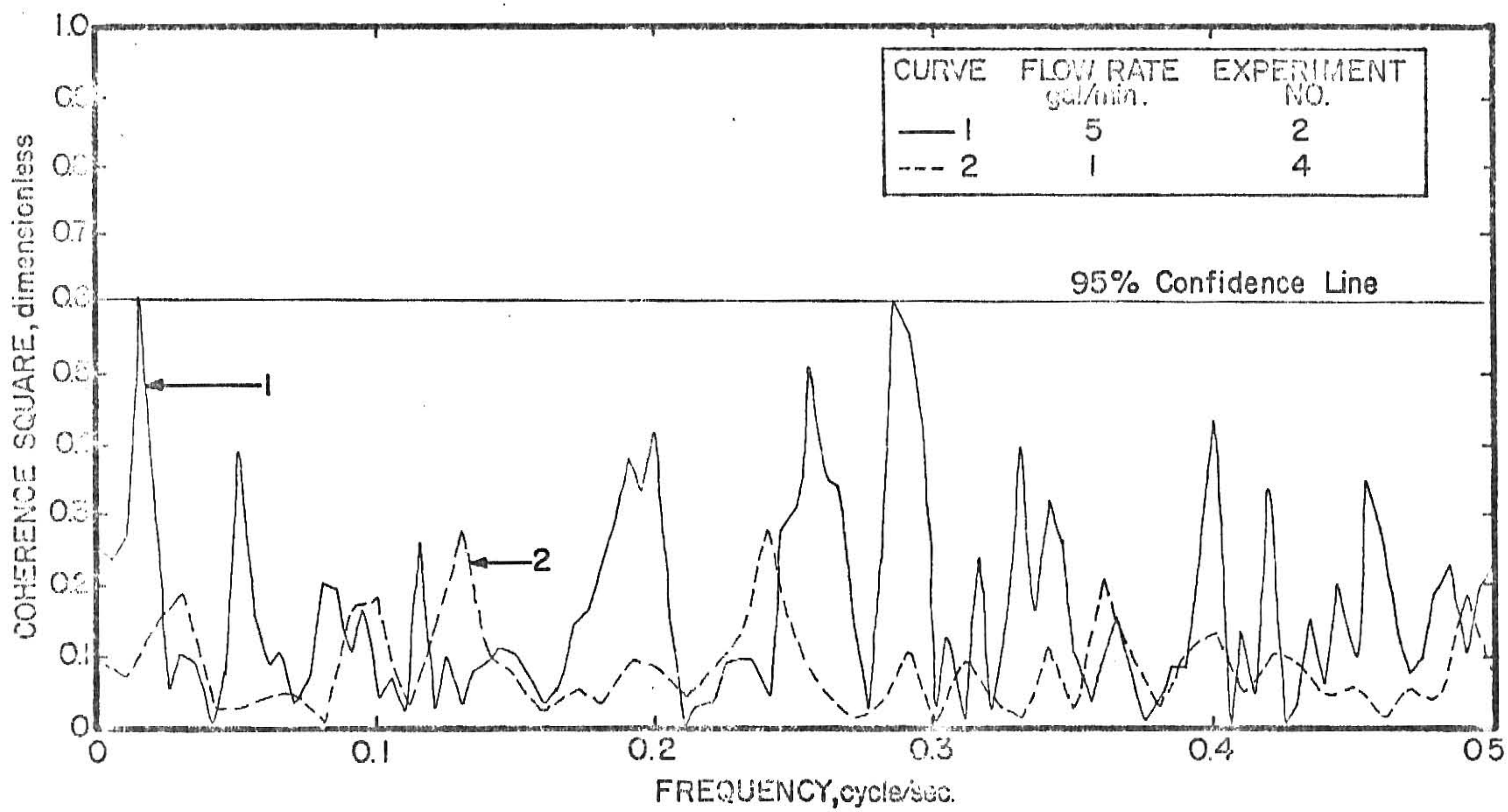

Fig.5.17. Effect of flow rate on coherence between middle and outlet temperatures for periodic steam input.

the autocorrelation and power spectrum at the middle temperature position. However, the visibility of the periodic thermal input in the downstream records decreases as the distance from the input increases and as the flow rate decreases. Examination of Fig. 5.15 shows moderately distinct peaks near the frequency of 0.05 cycles/sec for the middle and outlet temperatures in Experiment 4 (flow rate = 1 gal/min); however, the outlet temperature for Experiment 2 has a much larger peak at approximately 0.08 cycles/sec. As previously indicated, the record used to obtain Curve 1 is not stationary; thus, no significance should be attached to the peak at 0.08 cycles/sec. The normalized power spectrum results in Fig. 5.8 show a peak at 0.05 cycles/sec for subset 1 which is the stationary data set with small variance (0.0061). For subset 2 which has a much higher noise level (variance = 0.10) there is no peak at 0.05 cycles/sec even though this data set is stationary. It appears that the periodic thermal discharge is hidden by the high noise level in this particular case.

The position correlation results (Fig. 5.16) do not show any visible correlation between the middle and outlet temperatures. For Experiment 2, the correlation is positive at a lag of 30 seconds, but examination of the coherence and the components of the cross-spectrum indicates that no significant correlation exists between the data at the two positions. Figure 5.17 shows that the coherence is below the 95% confidence line at all frequencies. The amplitude of the transfer function appeared to be independent of frequency.

5.4 CONCLUSIONS

An experimental simulation of thermal discharge monitoring was carried out using two different stream flow rates and two types of thermal discharge. The responses to the monitored thermal inputs, measured at two different points along the stream, were analyzed by spectral analysis techniques. The effects of the periodic thermal input are observable in both the autocorrelation and power spectrum, The visibility of the periodic thermal input decreased as the distance from the input increases and as the flow rate decreases. A sampling point downstream but close to the point of discharge should be very useful in detecting periodic discharges into a stream. To extract more information from a stream affected by waste discharges, it is recommended that data be taken both upstream (Point B, Fig. 5.18) and downstream (Point C, Fig. 5.18) of the waste inputs.

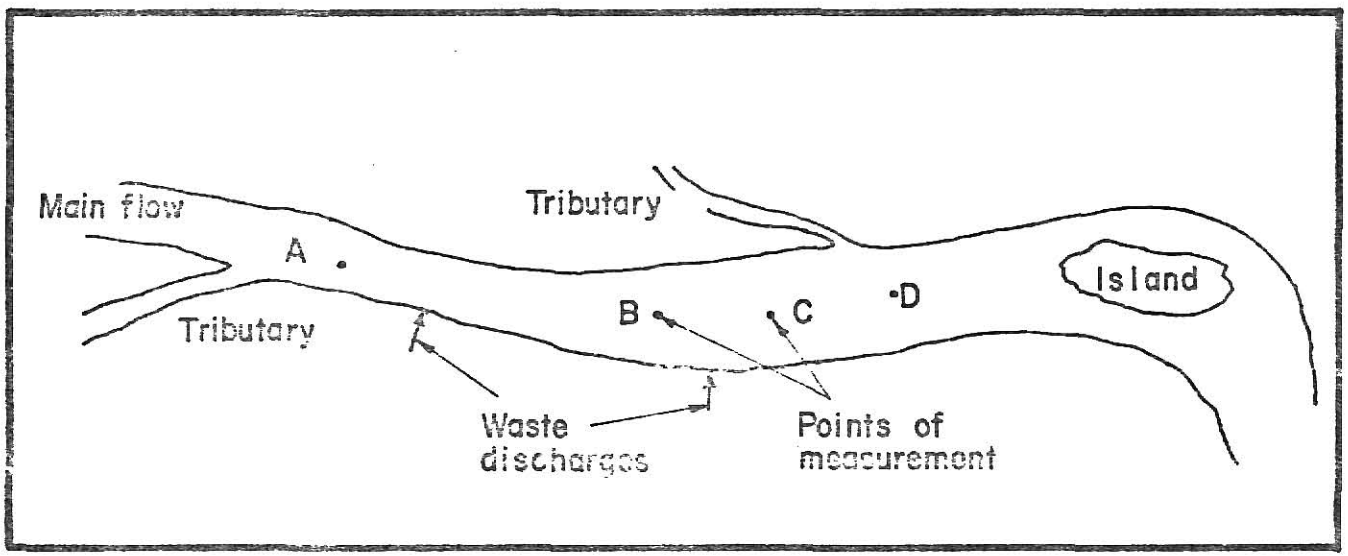

Fig.5.18. Selection of position of measurement to improve identification of events affecting water quality.

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CHAPTER 6

CONCLUSIONS AND RECOMENDATIONS

6.1 CONCLUSIONS

A new approach to estimate parameters in linear distributed parameter systems from time series data was developed in Chapter 3 of this dissertation. The advantage of this approach is that parameters may be estimated from experimental data collected at as few as two locations and using a minimum number of data points. Parameters appearing in a water quality model were estimated using this approach. The procedure is conceptually straightforward and can be conveniently implemented in linear time delay systems particularly when the system residence time is known. It was found in Chapter 4, that for a system with a noisy input Bard's method appeared to be the method of choice for estimating parameters; whereas for a system with noise corrupted measurements the Simplex method appeared to be the method of choice. This work also indicates that for a system with noisy input and noise corrupted measurements a search technique such as Simplex method would be a proper choice.

In the latter part of this dissertation, the responses to known (continuous and periodic) thermal inputs measured at two different points along a stream, were analyzed by spectral analysis techniques. The effects of the periodic thermal input were observable in both the autocorrelation and power spectrum. The visibility of the periodic thermal input decreased as the distance from the input increases and as the flow rate decreases. It was suggested that to extract maximum information from a stream affected by waste discharges the monitoring stations should be located at both upstream and downstream of the waste inputs.

In summary, the results obtained in this work may be used to develop a methodology to optimize the number of monitoring stations, the location of monitoring stations, and the amount of data required for analysis of water quality.

6.2 RECOMENDATIONS

There are several problems that seem to merit further consideration. These problems might include:

1. Development of sequential estimation procedures for updating values of the parameters in a continuous fashion.
2. The sensitivity of the parameters to fluctuations in waste and thermal discharge should be investigated. This information may be useful in detecting discharge violations in streams.

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ANALYSIS AND INTERPRETATION OF STOCHASTIC WATER QUALITY DATA USING PARAMETER ESTIMATION AND SPECTRAL ANALYSIS TECHNIQUES

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This thesis is concerned with the analysis and interpretation of stochastic water quality data. Spectral analysis and nonlinear parameter estimation techniques are employed to analyze the nature of stochastic events affecting water quality and their influence in the various water quality data and parameters.

An approach was presented for the identification of parameters in transient BOD and DO models. The models were plug flow models described by linear first-order partial differential equations. The approach was to reduce the partial differential equations to a set of ordinary differential equations with the method of characteristics from which an analytical solution was obtained. The time-lag phenomenon presented in plug flow models was exploited to correlate input-output data. A gradient method (Bard's method) and a Simplex pattern search technique were employed to identify parameters in the correlation equation. A system with noisy input, a system with noisy measurements and a system with noisy input and noisy measurements were considered in the identification problem.

Experimental data on stream temperature obtained from a laboratory model were used to illustrate the application of spectral analysis techniques to analyze noisy water quality data. Cyclic and continuous non-cyclic thermal discharges, superimposed on the inherently noisy signals of the stream, are used to generate the noisy data. The cyclic nature of the periodic thermal discharge could be observed. The applicability of these results to water quality monitoring is discussed. Finally, recomendations are made for future work in this area.