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ABSTRACT

Title of Thesis: A DYNAMIC MODEL OF A FILL-AND-DRAW
REACTOR UTILIZING AN INHIBITORY
SUBSTRATE

Yun-Fei Ko , Master of Science in Chemical Engineering,
1989

Thesis directed by: Dr. Gordon Lewandowski and
Dr. Basil C. Baltzis

A dynamic model of a fill-and-draw reactor has been developed, which includes a number of operational parameters, the fraction of total cycle time devoted to fill, reaction and draw, and the concentration of the toxic substance in the feed to the reactor.

Operating diagrams have been generated, from which one can choose suitable operating parameters.

The model has been solved numerically for Andrews kinetics (substrate inhibition), and tested experimentally, using a 5-liter fill-and-draw reactor with phenol as sole carbon source and a pure culture of Pseudomonas putida. Results compared very well to the model predictions.

A DYNAMIC MODEL OF FILL-AND-DRAW REACTOR
UTILIZING AN INHIBITORY SUBSTRATE

BY
Yun-Fei Ko

Thesis submitted to the Faculty of the Graduate School
of the
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of
Master of Science in Chemical Engineering

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I. INTRODUCTION

Control problems in biological processes are unique and oftentimes difficult because of the involvement of living organisms, which require the physical and chemical environment be controlled within narrow limits.

The performance of many processes and operations can be improved appreciably by controlled unsteady-state operations (periodic processes) [1,2]. In many cases it has been shown that processes operated periodically have much better results than those of conventional continuous flow operations. However, in the field of wastewater treatment, the continuous flow system (CSTR) has dominated the technology and fill - and - draw reactors have yet to gain wide acceptance. This was originally due to a lack of aeration equipment that would resist plugging during start / stop operation, labor costs associated with maintenance and supervision, and the perceived advantages of continuous processes. However, computer-aided operation of biochemical processes and new techniques in process control, have made fill-and-draw reactors competitive [3].

Fill-and-draw reactors (also known as semibatch or sequencing batch reactors) include fill, react, settle, draw, and idle periods, and may be composed of one or more reactors in series. Flexibility of operation allows those reactors to better accommodate variable wastes. Furthermore, since the reaction phase is mainly in a batch mode, the reaction products can be held in the reactor until they are acceptable for discharge. Other operational advantages of a fill-and-draw reactor include the capability of having both anoxic and aerated periods, and elimination of an external clarifier and sludge recycle [4], and a much smaller reactor volume for the same throughput [3].

II. LITERATURE REVIEW

Hsu [5] compared the performance of a 3.5 liter SBR with a 4-liter conventional activated sludge unit, using a petrochemical wastewater. Both the conventional unit and the SBR were operated at the same hydraulic retention time of about 10 days. During the fill phase, the feed was instantly added to the drawn-down reactor contents, and so the SBR was simply modelled as a batch reactor, using Monod kinetics. Both the SBR and conventional reactor were shock loaded with phenol at concentrations as high as 2000 ppm. The MLSS concentration was higher in the SBR, and the soluble BOD5 and nitrogen in the effluent were lower. However, more pin flocs were observed in the SBR, which contributed to a higher suspended solids concentration in the overflow. This may have been caused by the rapid method of feed addition. Although filamentous growth was clearly present in the conventional unit, its effect was mitigated by an oversized clarifier and a high sludge return rate. There was no filamentous growth in the SBR. The superior performance of the

SBR was observed in spite of the fact that a more efficient air diffuser was used in the conventional activated sludge unit.

While phenol degradation can be described by a Monod model at concentrations below 60 ppm [3], it is inhibitory above about 150 ppm, requiring an inhibition (Andrews) model [7, 8, 9, 10, 11].

Sokol and Howell [6] examined the biodegradation of phenol using pure cultures of Pseudomonas putida growing in continuous culture. Both Monod and Andrews models (as well as modifications there of) were applied to the data and the best fit kinetic parameters determined by regression.

Yang, and Humphrey [7] studied the microbial degradation of phenol by pure and mixed cultures of Pseudomonas putida both in batch and continuous culture systems. From these experiments, a kinetic model was developed and an analysis performed of the dynamic behavior of the system. The results

indicate that it should be possible to achieve effluent phenol concentration of 1 to 2 ppm in a single stage system . However, because of the effects of substrate inhibition, long lasting transients can occur. The transient behavior of such systems cannot be solely determined from the maximum specific growth rate and saturation constant, but must also include a consideration of the response characteristics of the microorganisms.

Rozich, Gaudy, and D'Adamo [8] also studied phenol degradation by an acclimated mixed microbial population. Various sources of seed populations were employed, and batch growth curves were generated using phenol as sole carbon source. An examination of 113 growth curves using five different inhibition functions failed to distinguish a function which was statistically superior to the others. Since the Andrews equation proved to be the most readily adaptive to curve-fitting procedures, it was selected as the best representation of the experimental data. Analysis of chemostat performance using growth constants determined in separate batch studies showed that batch growth data

can be used for prediction of activated sludge reactors treating toxic wastes.

The primary investigator responsible for rescuscitating fill-and-draw technology has been Robert Irvine at University of Notre Dame. Simulation studies of sequencing batch reactors were conducted by Irvine and Richter [9,10,11,12]. They developed design equations and obtained experimental data in a 4-liter bench-scale reactor using a synthetic industrial waste with a soluble TO of approximately 500 ppm. Computer simulation studies showed how the design volume for a fill-and-draw system varied with the mass flow rate.

Dennis and Irvine [13] studied the effect of fill time vs. react time on sequencing batch reactors. The influent feed concentration had a BOD5 of 400 ppm, the total cycle time was 8 hours, and the volume of the reactor was 4 liters. They found that the average effluent BOD5 was 3 ppm in all cases. They also concluded that a semi-batch reactor can achieve higher effluent quality than a CSTR of similar size.

Chiesa and Irvine [14] concluded that intermittent feeding patterns impose growth conditions most favorable for micro-organisms physiologically characterized as having high rates of substrate assimilation and high resistance to starvation. This type of organism selection is particularly applicable to low net growth systems such as the activated sludge process. Filamentous organisms responsible for many of the reported incidences of bulking lack either one or both of these important traits, and their numbers can be controlled by engineering a system to provide a properly balanced feed pattern. Continuous flow reactors can also be designed and operated to control filamentous growth, although the range over which these systems can be reliably operated is narrower than that for intermittently fed systems operated under the same general conditions.

Bell and Hardcastle [15] studied the treatment of munitions plant waste. A bench-scale continuously fed, intermittently operated activated sludge system was operated for more than 30 months. Various operating protocols were used. Organic removal was consistently

high and nitrification and denitrification were essentially complete. Because of the light nitrogen loading nitrification and denitrification rates were low. Solids separation was good throughout the study. The system was highly stable and extremely tolerant of changes in operating conditions, including shocks from power outages, mixer failure, and accidental over-feeds.

Hoepker and Schroeder [16] studied the effect of loading rate on activated sludge effluent quality. Their experiments consisted of two types of reactors : batch (0 fill time) and semi-batch (8-hour fill time). They pointed out that for lower feed concentration and flow, semi-batch operation had better effluent quality and was considerably more stable in terms of dispersed growth, even though a relationship with growth rate could not be established.

Ketchum, Irvine, and Lias [17] studied the cost analysis of sequencing batch biological reactors. They concluded that the sequencing batch system, required the least cost of the alternatives considered for small facilities in small rural communities.

III. OBJECTIVES

In previous work [3], the mathematical model using Monod kinetics has been verified experimentally. It showed very good agreement between theory and experiment, when the phenol concentration was lower than 60 ppm. On the other hand, when the substrate concentration was higher than 100 ppm, substrate inhibition occurred, which was not accounted for by the Monod model. Hence, the substrate inhibition case still needed further study.

In the present work, parameters were determined for the Andrews model (substrate inhibition), and the model was verified experimentally.

IV. MATHEMATICAL MODEL

A detailed mathematical model has been derived in dimensionless form describing the operation of the SBR. The formulation of the model is such that it allows the performance of the SBR to be easily compared to an equivalent continuous stirred tank reactor (CSTR). The model has been derived and solved for Andrews (inhibitory) kinetics. The model assumes that the duration of the settling and idle phases is negligible relative to that of the other three phases (fill, react, draw) and thus can be neglected. Furthermore, the model assumes that biodegradation (reaction) occurs during all three phases (fill, react, and draw). Figure 1 shows a qualitative diagram of the change in the working volume of the reactor as a function of time.

DERIVATION OF THE MATHEMATICAL MODEL

(1) General

The equations describing the system at any instant of time are the following:

$$\frac{dV}{dt} = Q_f - Q \quad (1)$$

The equation above is written under the assumption of constant density. The symbols appearing in equation (1) are defined as follows:

V = working volume of the reactor

Q_f = volumetric flow rate of the stream fed into the reactor

Q = volumetric flow rate of the stream exiting the reactor

Mass balance on the biomass:

$$\frac{d(Vb)}{dt} = Q_f b_f - Qb + \mu(s)bV$$

or

$$V \frac{db}{dt} + b \frac{dV}{dt} = Q_f b_f - Qb + \mu(s)bV$$

or, by using equation (1)

$$\frac{db}{dt} = \frac{Q}{V} (b_f - b) + \mu(s)b \quad (2)$$

The symbols appearing in equation (2) and not introduced before, are defined as follows:

b = concentration of biomass in the reactor and in the stream exiting the reactor

b_f = concentration of biomass in the feed to the reactor. For all practical purposes, unless there is recycle of solids to the reactor, the value of this quantity is zero.

$\mu(s)$ = specific growth rate of the biomass. It is a function of the concentration of the hazardous or toxic substance which exerts rate limitation on growth.

Mass balance on the rate-limiting substrate (i.e., on the toxic substance which is treated in the unit)

$$\frac{ds_f}{dt} = \frac{Q}{V} (s_f - s) - \frac{\mu(s)b}{Y} \quad (3)$$

The symbols not previously introduced and appearing in equation (3) are defined as follows:

s_f = concentration of the toxic substance in the waste fed into the reactor.

s = concentration of the toxic substance in the reactor and in the stream exiting the reactor.

Y = yield coefficient of the biomass on the toxic substance. It stands for the efficiency with which the biomass converts the substrate into more biomass. The yield is assumed to be constant.

Clearly, some of the terms appearing in equations (1) through (3) are zero during some of the phases of operation. For instance, there is no input or output from the reactor during the reaction phase. This becomes clear in the following sections when each phase of operation is described separately.

(2) Use of Andrews Kinetics

The Andrews model sometimes referred to as the Haldane model, expresses the specific growth rate as follows:

$$\mu(s) = \frac{\mu_s}{k_s + s + \frac{s^2}{k_i}}$$

where,

μ = characteristic constant having units of
inverse time

k_s = constant having units of concentration

k_i = inhibition constant of the population

μ , k_s , and k_i are parameters characteristic of the particular substrate and of a given population.

Equations (1) through (3) can be written in dimensionless form as follows :

$$\frac{dV}{d\theta} = Q'_f - Q' \quad (4)$$

$$\frac{dx}{d\theta} = \frac{Q'_f}{V'} (x_f - x) + \frac{u}{1 + u + \gamma u^2} \beta x \quad (5)$$

$$\frac{du}{d\theta} = \frac{Q'_f}{V'} (u_f - u) - \frac{u}{1 + u + \gamma u^2} \beta x \quad (6)$$

where

$u = \frac{s}{k_s} =$ dimensionless concentration of the toxic
substance in the reactor and in the
stream exiting the vessel.

$$u_f = \frac{s_f}{k_s} = \text{dimensionless concentration of the toxic substance in the stream fed into the reactor.}$$

$$x = \frac{b}{Yk_s} = \text{dimensionless biomass concentration of the biomass in the reactor and in the reactor exit.}$$

$$x_f = \frac{b_f}{Yk_s} = \text{dimensionless biomass concentration in the stream fed into the reactor}$$

(x = 0 in most case).

$$Q'_f = \frac{Q_f}{Q_r} = \text{dimensionless volumetric flow rate of the stream fed into the reactor (} Q_r \text{ is a reference volumetric flow rate defined later in this section).}$$

$$Q' = \frac{Q}{Q_r} = \text{dimensionless volumetric flow rate of the stream leaving the reactor.}$$

$$V'_r = \frac{V_r}{V_r} = \text{dimensionless working volume of the reactor}$$

(V_r is a reference volume defined later in this section).

$$\theta = \frac{tQ_r}{V_r} = \text{dimensionless time.}$$

$$\beta = \frac{\mu V_r}{Q_r} = \text{dimensionless hydraulic residence time of an equivalent CSTR.}$$

$$\gamma = \frac{k_s}{k_i} = \text{dimensionless inverse inhibition constant.}$$

(3) Description of an Equivalent CSTR

One of the objectives of this analysis is to quantitatively compare the operational efficiency of the SBR to that of a CSTR, so one has to mathematically describe the latter as well as the former.

The SBR, as discussed above, is described by equations (4) through (6). In the SBR things change continuously with time, while a CSTR operates at steady state. The CSTR is also described by equations (4) through (6), provided that the left hand side of these equations is set equal to zero (i.e., no change with time). Hence,

$$Q'_f - Q' = 0 \quad (7)$$

$$\frac{Q'_f}{V'} (x_f - x) + \frac{u}{1 + u + \gamma u^2} \beta x = 0 \quad (8)$$

$$\frac{Q_f}{V'} (u - u) - \frac{u}{1 + u + \gamma u^2} \beta x = 0 \quad (9)$$

Q_r and V_r (introduced before) are defined as the volumetric flow rate of the stream continuously fed into the CSTR, and the volume of the CSTR, respectively. Then, in the case of the CSTR:

$$Q'_f = Q'_r = V'_r = 1$$

solving equations (8) and (9), one gets:

$$x = u_f + x_f - u_f \quad (\text{known as the stoichiometric relation})$$

Since in most cases $x_f = 0$

$$x = u_f - u_f \quad (10)$$

$$u = \frac{\beta - 1 - [(\beta - 1)^2 - 4\gamma]^{0.5}}{2\gamma} \quad (11)$$

Expressions (10) and (11) are for the case where no biomass is fed into the CSTR. Furthermore the analysis has revealed the following:

(a) If

$$u_f < \left[\frac{1}{\gamma} \right]^{0.5}$$

the CSTR can not function unless

$$\beta > 1 + \gamma u_f + \frac{1}{u_f}$$

In case the latter condition is violated, the biomass washes-out of the reactor.

(b) If

$$u_f > \left[\frac{1}{\gamma} \right]^{0.5}$$

the CSTR can never be operated at $\beta < 1 + 2\gamma^{0.5}$, since in such cases the biomass always washes-out.

(c) If

$$\beta > 1 + \gamma u_f + 1/u_f$$

the CSTR can be always safely operated.

(d) If

$$1 + \gamma u_f + 1/u_f > \beta > 1 + 2\gamma^{0.5}$$

the CSTR can lead either to culture washes-out or to proper operation. The outcome depends on how one starts up the reactor (i.e., on initial biomass and substrate concentration) and also on an appropriate process control system capable of damping any significant perturbations since in the region of the double inequality, reactor operation is not globally stable.

The conversion of the toxic substrate achieved with a

CSTR is defined as:

$$Y = \frac{u_f - u}{u_f}$$

or by using relation (11)

$$Y = \frac{2\gamma u_f + 1 - \beta + [(\beta - 1)^2 - 4\gamma]^{0.5}}{2\gamma u_f} \quad (12)$$

(4) Description of the Phases of the SBR

Figure (1a) indicates the way the volume of the system changes with time during the various phases. V_{\max} is the maximum working volume, (i.e., the volume of the system at the end of the fill phase), while V_0 is the volume of the system at the end of the draw phase.

During the fill phase ($0 \leq t \leq t_1$), the volume increases linearly with time since the system is fed at a constant volumetric flow rate. During the react phase ($t_1 \leq t \leq t_2$), as well as during the settle phase ($t_2 \leq t \leq t'_2$), the volume of the system remains constant and equal to V_{\max} . During the draw phase ($t'_2 \leq t \leq t_3$), the volume of the system decreases linearly with time (because the reactor

is emptied at a constant flow rate) from the value V_{\max} to the original value V_0 . During the idle phase ($t \leq t \leq t'$), the volume of the system remains constant and equal to V_0 . At time $t=t'$, the cycle is repeated.

The diagram shown in Figure (1b) indicates the way the volume of the system is assumed to change with time in the present study, in which no settle or idle periods are considered.

The volume and volumetric flow rates appearing in equations (1) through (3) can be expressed as follows for the various phases:

(a) Fill phase ($0 < t \leq t_1$)

$$Q_f = Q_{f,SBR} ; Q = 0 ; V = V_0 + Q_f t$$

where $Q_{f,SBR}$ is the volumetric flowrate of the feed to the SBR, and it is more specifically defined later in this section.

(b) React phase ($t_1 \leq t \leq t_2$)

$$Q_f = 0 ; Q = 0 ; V = V_{\max}$$

(c) Draw phase ($t_2 \leq t \leq t_3$)

$$Q_f = 0 ; Q = Q_{f,SBR} ; V = V_{\max} - Q_{f,SBR}(t - t_2)$$

As discussed previously, the results of the analysis are to be used in order to compare the performance of an SBR to that of a CSTR. The comparison will be valid only if it is based on equivalent quantities. Hence, the volume of the CSTR, and V_{\max} of the SBR, must be the same so that the comparison is based on vessels of the same volume. Both vessels must also have the same time-average throughput of process material (i.e., same volume of feed processed by both reactors per unit time). In view of the foregoing arguments, one can write:

$$V_r = V_{\max} \quad (13)$$

$$[Q]_r t_3 = [Q]_{f,SBR} t_1 \quad (14)$$

It is also true (under the assumption of constant density) that the volume fed into the SBR during the fill phase must be equal to the volume exiting the SBR during the draw phase, i.e.,

$$[Q]_{f,SBR} t_1 = Q[t_3 - t_2] \quad (15)$$

By defining,

$$\sigma_1 = \frac{t_1}{t_3} = \text{fraction of total cycle time devoted to the fill phase.}$$

$$\sigma_2 = \frac{t_2 - t_1}{t_3} = \text{fraction of total cycle time devoted to the react phase.}$$

$$\sigma_3 = \frac{t_2 - t_3}{t_3} = \text{fraction of total cycle time devoted to the draw phase.}$$

and using relations (14) and (15) it is clear that

$$Q'_f = Q_{f, \text{SBR}} = \frac{1}{\sigma_1}, \text{ and } Q'_r = \frac{1}{\sigma_3} \quad (16)$$

At the end of the fill phase, the volume of the reactor reaches its maximum value, V_{max} (or V_r by equation (13)), and thus, one can write

$$1 = \delta = Q'_f \vartheta_1$$

or by using the first relation (16)

$$1 = \delta + \frac{1}{\sigma_1} \vartheta_1, \text{ or } \vartheta_1 = (1 - \delta)\sigma_1 \quad (17)$$

where
$$\delta = \frac{V_0}{V_{\text{max}}}$$

i.e., the fraction of the vessel which is occupied by mixed liquor at the end of the draw phase.

From the definition of σ_3 , one can see that

$$\sigma_3 = \frac{v_3 - v_2}{v_3} \quad (18)$$

At the end of the draw phase, the volume of the system is equal to its minimum value, V_0 , and thus one can write

$$\delta = 1 - Q' \left(\frac{v_3 - v_2}{v_3} \right)$$

or by using the second relation (16)

$$\delta = 1 - \frac{1}{\sigma_3} (v_3 - v_2) \quad (19)$$

Combining relations (18) and (19), one gets

$$v_3 = 1 - \delta \quad (20)$$

Relations (19) and (20) also result in

$$v_2 = (1 - \delta)(1 - \sigma_3) \quad (21)$$

Using relations (16), (17), (20) and (21) one can now describe the volumetric flow rate and the volume of the system during the three phases as follows:

$$\text{fill phase, } 0 < v \leq (1 - \delta)\sigma_1$$

$$Q'_f = \frac{1}{\sigma_1}; \quad Q' = 0; \quad V' = \delta + \frac{1}{\sigma_1} v$$

react phase, $(1 - \delta)\sigma_1 \leq \vartheta \leq (1 - \delta)(1 - \sigma_3)$

$$Q'_f = 0 ; Q' = 0 ; V' = 1$$

draw phase, $(1 - \delta)(1 - \sigma_3) \leq \vartheta \leq 1 - \delta$

$$Q'_f = 0 ; Q' = \frac{1}{\sigma_3} ; V' = 1 - \frac{1}{\sigma_3} [\vartheta - (1 - \delta)(1 - \sigma_3)]$$

In view of the above, equations (4) through (6) can be written as follows:

fill phase, $0 < \vartheta \leq (1 - \delta)\sigma_1$

$$\frac{du}{d\vartheta} = \frac{1}{\delta\sigma_1 + \vartheta} (u_f - u) - \frac{u}{1 + u + \gamma u^2} \beta x \quad (22)$$

$$\frac{dx}{d\vartheta} = \frac{1}{\delta\sigma_1 + \vartheta} (x_f - x) + \frac{u}{1 + u + \gamma u^2} \beta x \quad (23)$$

react and draw phases, $(1 - \delta)\sigma_1 \leq \vartheta \leq 1 - \delta$

$$\frac{du}{d\vartheta} = -\beta x \frac{u}{1 + u + \gamma u^2} \quad (24)$$

$$\frac{dx}{d\vartheta} = \beta x \frac{u}{1 + u + \gamma u^2} \quad (25)$$

In the formulation of the problem presented here, it has been assumed that reaction (biodegradation) occurs not only during the react phase, but during the fill and draw phases as well.

In the original formulation of the problem (equations (1) through (3)), one needs to specify the values of 11 parameters in order to solve the equations and predict the behavior of the system. These parameters are V_0 , t_1 , t_2 , t_3 , μ , k_i , k_s , Y , s_f , b_f and Q_f .

The values of V_{max} and Q are not independent parameters, since $V_{max} = Q_f t_1 + V_0$ and $Q(t_3 - t_2) = Q_f t_1$. In the final formulation of the problem (equations (22) through (25)) in terms of the dimensionless quantities (u and x), one needs to specify the values of 6 parameters (i.e., x_f , u_f , σ_1 , σ_3 , γ , and δ). This reduction in the number of the parameters from 11 to 6, reduces tremendously the amount of numerical work which needs to be done in order to study the behavior of the system in full detail.

(4) Conversion Achieved by the SBR and Relative Yield

The conversion of the toxic substrate achieved by the SBR is defined as follows:

$$Y_{\text{SBR}} = 1 - \frac{A}{B} \quad (26)$$

where, A = the amount of unconverted substance per cycle

B = the amount of toxic substance fed into the reactor per cycle

In terms of dimensional quantities, A and B are given by the following expressions:

$$A = \int_{t_2}^{t_3} Q_s dt ; B = \int_0^1 Q_{f,\text{SBR}} s dt = Q_{f,\text{SBR}} s t$$

In terms of dimensionless quantities, A and B are given by the following expressions:

$$A = \frac{1}{\sigma} \int_{\frac{1}{3}}^{(1-\delta)} \frac{(1-\delta)}{(1-\delta)(1-\sigma)} u d\theta ; B = u_f (1 - \delta)$$

During transient cycles the conversion changes, but when the system reaches its limit cycle or steady operation, the conversion is constant. The end of the transient cycles is reached when the value of u at any time θ is

equal to that at time $\theta + N(1-\delta)$, where N is any integer number.

The comparison of the performance of the SBR to that of an equivalent CSTR is quantitized by the relative yield ϵ as:

$$\epsilon = \frac{y_{\text{SBR}}}{y} \quad (27)$$

where y is the conversion achieved with the SBR and y_{SBR} is the conversion achieved with an equivalent CSTR. The value of y is calculated from the expression (12) (no biomass is assumed to be fed into the reactor). The value of y_{SBR} in expression (27) is calculated from expression (26) for the steady conditions (i.e., after the decay of all transients).

V. EXPERIMENTAL APPARATUS

A. Batch System

All experiments were conducted at room temperature (approximately 26 °C). The inoculated solutions were placed in 250 ml flasks on a rotary shaker (model G-24 New Brunswick Scientific Company, New Brunswick, NJ). There were no baffles. No air other than that transferred by shaking was provided.

B . SBR System

All experiments were conducted at room temperature (approximately 26 °C). The reactor was a 15 cm diameter, 5-liter capacity, cylindrical vessel structured of Lucite, capped with a removable lid. An effluent port was installed two liters above the bottom, with a solenoid valve to control the discharge of treated wastewater.

Aeration alone provided the agitation and there was no mechanical stirring.

Laboratory compressed air was passed through a series of filters and activated carbon before entering the reactor. The volume of air was regulated

by two needle-valve rotameter, with a solenoid valve on each air line. To increase the efficiency of air/liquid contact, an aquarium diffuser stone was placed on the end of each air line at the bottom of the reactor.

A microprocessor (Omron, Sysmac-PO Sequence controller) controlled the system (feed peristaltic pump, air solenoid valves, and decant solenoid valve). Any combination of fill, react, settle, and draw period times could easily be programmed into the computer. The output setting and programming of the sequence controller are described in Appendix A.

A schematic diagram of the fill-and-draw reactor assembly is depicted in Figure 2.

C. Analytical Equipment

(1) Varian Model 3370 Gas Chromatograph with flame

Ionization detector

operating temperatures

oven = 140 °C

injector port = 210 °C

detector = 250 °C

- (2) GC column - 6 ft x 1/8", ss, 10 % sp-2100 on 100/120 Supelcoport.
- (3) Hewlett-packard 3390 Electronic Integrator
- (4) DO & PH meter Orion Research, Model 701 A
- (5) DO & PH recorder Kipp & Zonen, Model BD 401
- (6) DO electrode Orion Research, Model 97-08
- (7) PH electrode Orion Research, Model 91-04
- (8) Spectrophotometer Bausch & Lomb, Spectronic 20

VI. EXPERIMENTAL PROCEDURES

In order to have a clear test of the mathematical model, it was necessary to obtain well defined, constant, rate parameters for the microbial population employed in the reactor. As a result, a pure culture of Pseudomonas putida (ATCC 31800) was used in this study. Its growth parameters were obtained and the model was tested against the pure culture performance in the SBR.

A stock culture was maintained by periodic subculture on Difco-Bacto nutrient broth and stored at 4°C in a refrigerator. The primary culture was prepared by transferring a loop of stock culture to 2.5 ml of sterilized defined medium solution diluted with 47.5 ml of distilled water (i.e., a final concentration of 50 ppm phenol). The inoculated culture was then placed in a 250 ml flask and incubated for approximately one day at 28 °C in a rotary shaker bath (rotating at 250 rpm). The medium was aerated by virtue of the shaking process.

A secondary culture was prepared by transferring 2.5 ml of sterilized defined medium solution diluted with 45 ml of distilled water. The inoculated culture was then placed in a 250 ml flask and incubated for 12 to 14 hours

at 28°C in a rotary shaker bath (rotating at 250 rpm). The medium was aerated by virtue of the shaking process.

This procedure was repeated for a tertiary culture in order to insure that the culture had fully adapted to growth on the phenol medium and that phenol was the sole carbon source.

A. Formulation of Defined Medium

Many formulations of medium solutions have been proposed for which there is often little or no fundamental justification [18]. The composition of the phenol defined medium solution used in the present study (Table 1) has been suggested by Gaudy [19], which contained carbon, nitrogen and phosphate as nutrients. Phenol was the sole carbon source and ammonium sulfate/potassium phosphate provided nitrogen, phosphorus and buffer.

B. Determination of Andrews Parameters

Pure culture growth parameters were obtained from batch

experiments on tertiary cultures in shaker flasks [3,20]. This involved measuring the optical density of the culture on exposure to different initial concentrations of phenol (Table 2). When the phenol concentration is high (e.g., 140 , 180 , 220 ppm etc.), one needs to take a lot of samples (it takes a long time for the microbes to degrade the phenol), hence , a pre-run is required in order to a get rough idea of the growth behavior of the Pseudomonas putida, and minimize the amount of liquor removed from the reactor. Pre-runs were made at initial phenol concentrations of 20, 120, and 220 ppm. The minimum required sampling volume with the Spectronic 20 for measuring the optical density is 2.5 ml. From the pre-run data, for phenol concentrations of 20 and 60 ppm, samples were taken every 20 to 30 minutes; while at phenol concentrations of 100, 140, 180, and 220 ppm, samples were taken after 3 hours, 2 hours, and then every hour.

The optical density could be converted to biomass. (Table 3) using a calibration curve (Figure 3), and the initial slope determined on a semi-log plot (Figures 4-1 to 4-6, Figures 5-1 to 5-6, Figures 6-1 to 6-6). The initial slope is the specific growth rate, which could then be plotted versus the initial phenol concentrations.

In addition, the yield coefficient Y was determined by plotting the biomass concentration (Table 3) versus phenol concentration (Table 4), as indicated in Figures 7-1 to 7-6, Figures 8-1 to 8-6, and Figures 9-1 to 9-6.

C. Numerical Methods

A standard procedure of the least squares method was applied in order to get the Andrews parameters (μ , k_s , k_i). The augmented jacobian matrix used in the method is the following:

$$\begin{bmatrix} A(1,1) & A(1,2) & A(1,3) & A(1,4) \\ A(2,1) & A(2,2) & A(2,3) & A(2,4) \\ A(3,1) & A(3,2) & A(3,3) & A(3,4) \end{bmatrix}$$

where

$$A(1,1) = \sum_{I=1}^6 2 \left[\frac{s(I)}{\Delta} \right]^2$$

$$A(1,2) = \sum_{I=1}^6 2 \frac{s(I)}{\Delta} \left[u(I) - 2 \frac{\mu s(I)}{\Delta} \right]$$

$$A(1,3) = \sum_{I=1}^6 \frac{2s(I)^3}{(k \Delta)_i^2} \left[\frac{\mu s(I)}{\Delta} - u(I)^2 \right]$$

$$A(1,4) = \sum_{I=1}^6 \frac{s(I)}{\Delta} \left[u(I) - \frac{\mu s(I)}{\Delta} \right]$$

$$A(2,1) = \sum_{I=1}^6 \frac{2s(I)}{\Delta} \left[u(I) - \frac{2s(I)\mu}{\Delta} \right]$$

$$A(2,2) = \sum_{I=1}^6 \frac{2s(I)\mu}{\Delta^3} \left[\frac{3s(I)\mu}{\Delta} - 2u(I) \right]$$

$$A(2,3) = \sum_{I=1}^6 \frac{2s(I)\mu}{(k \Delta)_i^2} \left[2u(I) - \frac{\mu 3s(I)^2}{\Delta} \right]$$

$$A(2,4) = \sum_{I=1}^6 \frac{2s(I)\mu}{\Delta} \left[\frac{s(I)\mu}{\Delta} - u(I) \right]$$

$$A(3,1) = \sum_{I=1}^6 \frac{2s(I)^3}{(k \Delta)_i^2} \left[\frac{s(I)\mu}{\Delta} - u(I) \right]$$

$$A(3,2) = \sum_{I=1}^6 \frac{2\mu s(I)^3}{k_i \Delta^2} \left[2u(I) - \frac{3\mu s(I)}{\Delta} \right]$$

$$A(3,3) = \sum_{I=1}^6 \frac{2\mu s(I)^3}{(k_i \Delta)^3} \left\{ \mu s(I) \left(\frac{3s(I)^2}{k_i \Delta} - 2 \right) + u(I) \left[2(k_i + s(I)) \right] \right\}$$

$$A(3,4) = \sum_{I=1}^6 \frac{2\mu s(I)^3}{(k_i \Delta)^2} \left(u(I) - \frac{\mu s(I)}{\Delta} \right)$$

Symbols appearing in the elements of the Jacobian above, are defined as:

$$\Delta = k_s + s(I) + \frac{s(I)^2}{k_i}$$

$s(I)$ is the initial phenol concentration. (eg., $s(1) = 20$ ppm)

$u(I)$ is the specific growth rate which is evaluated at $s(I)$ phenol concentration.

D. SBR Experiments

In the sequencing batch experiments, 2 liters of diluted defined medium solution at the appropriate phenol concentration, were inoculated in the 5-liter Lucite reactor with the tertiary shaker flask culture. Growth was allowed to proceed in batch mode (periodically adding defined medium solution when the phenol was depleted), until the biomass concentration was between 30 and 140 % of its maximum steady cycle value, when survival was expected. Once this was achieved, the SBR sequence was initiated.

During the fill phase, the reactor contents were aerated to match the conditions of the mathematical model. The pumping rate was adjusted so that the reactor volume increased from 2 liters to 4 liters during the fill period. The aeration rate was undetermined, since it was above the highest rotameter setting (60 cc/min for each of two lines entering the reactor). The reason for this was to maintain a relatively constant DO level (about 7 ppm) in the reactor, the rotameters were undersized. It is estimated that the total aeration rate to the reactor was at least 300 cc/min.

DO and PH were monitored continuously with immersed electrodes and a two pen recorder. The DO dropped a few tenths of a ppm during fill, but generally held constant at about 7.

In the react phase, the feed pump was shut off, aeration was continued, and substrate and biomass samples were taken periodically.

At the end of the react phase, aeration was continued, and the decant solenoid valve was opened to completely discharge 2 liters of mixed liquor. By continuing aeration during discharge, there was a predicted loss of biomass, which was recovered by growth during the fill and react phases, in cases where the biomass was not eventually washed-out. This was done to simplify the reactor operation and make it easier to compare the results with the mathematical model. In a real operation, there would be a quiescent settling period prior to discharge.

At the end of an entire run, a nutrient agar plate was streaked to determine if any significant contamination had occurred. Visual inspection of the incubated colonies indicated only those of Pseudomonas putida.

E . Analytical Procedures

(1) Biomass Growth

For all experiments, the course of growth of the microorganisms was determined by the optical density of the mixed liquor, using a spectrophotometer at a wavelength of 540 nm and distilled water as the reference sample. The optical density was then converted to biomass concentration using a calibration curve (Figure 3) obtained earlier [20] and confirmed in this study through the following procedure:

Pseudomonas putida was grown in a standard nutrient broth, harvested towards the end of the logarithmic growth phase (after about two days), and serially diluted. The turbidity of each dilution (1/10, 2/10, 3/10, 4/10, 5/10) was determined spectrophotometrically.

For the dry weight determination of cell mass, three 10 ml samples were taken from the original culture solution (undiluted) and pipetted into three numbered, preweighed aluminum dishes. The water was then evaporated in an oven at 95 °C for 24 hours and the samples reweighed to determine the biomass concentration. The biomass concentrations of other serially diluted samples were

determined by dividing the dry weight value by each dilution ratio. The data points of the confirmation test are also shown in Figure 3, which shows very good consistency with the previous study.

For all experiments in this study, in order to avoid a significant reduction in volume caused by taking large samples from the reactor, 3 ml samples were taken each time (the minimum sample volume for measuring the optical density is 2.5 ml). Samples were taken periodically from the reactor and added to 10 ml cuvettes for immediate measurement of the optical density. The same samples were then used to measure the substrate concentration.

In handling the cuvettes, the following procedures were followed:

- a. The cuvettes were rinsed several times with distilled water to get them clean before use.
- b. The lower part of the cuvettes were kept spotlessly clean by keeping them free of liquids, smudges, and finger prints, and were wiped clean with lint-free tissue (not with towels or handkerchiefs).

After each sample the pipet was cleaned in order to avoid biomass attachment to the glass wall.

(2) Substrate Analysis

Right after the optical density was measured; the sample was analyzed immediately by gas chromatography (at least two times for each sample). 0.5 ml of a 500 ppm thymol solution were added to the cuvettes as an internal standard. The accuracy of the analysis was about +/- 1 ppm. In the batch experiments (phenol concentrations of 20, 60, 100, 140, 180, 220 ppm), the sampling order was from higher concentration to lower concentration. Distilled water blanks were injected into the gas chromatograph between samples.

VII. EXPERIMENTAL RESULTS AND DISCUSSION

Results for the specific growth rate, yield coefficient and Andrews parameters for Pseudomonas putida, utilizing phenol as the sole carbon source, are given in Tables 5, 6, and 7 (for phenol concentrations of 20, 60, 100, 140, 180, 220 ppm).

Pseudomonas putida exhibited substrate inhibition at phenol concentrations higher than 60 ppm (Figure 10). The average Andrews parameters (for triplicate runs) were $\mu = 1.395$ 1/hr, $k_i = 51.000$ ppm, $k_s = 47.101$ ppm, and $Y = 0.286$ mg biomass / mg substrate.

The pure culture was then utilized in the SBR for seven runs. The experimental conditions and results are shown in Tables 8 to 14.

All of the experimental conditions for the SBR were chosen based on the theoretical operating diagram (Figure 13).

Figures 13 to 42 compare the theoretical curves with the experimental points for the seven runs (at feed concentrations of 35 ppm, three at 100 ppm, and three at 140 ppm). The prediction from theory is as follows:

SBR1-35 ppm	survival
SBR2-100 ppm	survival
SBR3-100 ppm	washout
SBR4-100 ppm	survival (duplicate)
SBR5-140 ppm	survival
SBR6-140 ppm	survival
SBR7-140 ppm	washout

SBR5, SBR6 and SBR7 were running at the same β and u_f , but at different initial biomass concentrations (to test the validity of the operating diagram).

Figures 13, 14, 17, 18, 21, 22, 31, 32, 35, 36, 39 and 40 show results during a transient cycle. Figures 15, 16, 19, 20, 23, 24, 27, 28, 33, 34, 37, 38, 41 and 42 show the results of the steady cycle. It required 4 to 18 cycles to reach the steady cycle in the survival case, depending on how the experiment was started up. In the washout case, it might require more than 15 to 20 cycles to reach the steady cycle.

It is very difficult, when dealing with living organisms to account for, much less control, all of the possible variables in the system. Therefore, although there was a constant discrepancy for the biomass concentration, the

results still show very good agreement between theory and experiment.

Agreement with the shape of the transient curves is a strong indication of the validity of the mathematical model (both biomass and substrate concentration). In the steady cycle, one can observe that the substrate prediction is perfectly matched by the experimental data. But, there is a constant discrepancy between the theoretical prediction and the experimental data for the biomass. A likely explanation for this discrepancy is that Pseudomonas putida cells attached to the wall of the reactor, although no biofilm formation was observed. It was observed though that the diffuser stone, after several cycles, became brown, indicating attachment of biomass on it.

In order to check cell wall attachment, an experiment was run with the following procedure:

- a. After the steady cycle, the reactor was drained, then 4 liters of distilled water were added to the reactor, and drained again.
- b. 4 liters of growth medium (phenol concentration = 40 ppm) were then added to the reactor.
- c. After two to three days, the phenol concentration dropped below 3 ppm.

The experiment above proved that wall attachment actually occurs and that it may account for the discrepancy between the theoretical predictions and experimental data for biomass concentration.

Another possible explanation for the discrepancy between predicted and actual biomass is the endogenous requirement of the Pseudomonas putida. Both experiments and computer simulations were performed to test this assumption.

In the experiments, 100 ml of mixed liquor (i.e., 5 ml of tertiary culture, 5 ml of 1000 ppm growth medium, and 90 ml of autoclaved-distilled water) were added to a 250 ml flask. The flask was put in the shaker, which was operated at 28 °C, and 250 rpm. After the specific growth rate leveled off, samples were taken every 40 to 50 minutes for 5 hours. It was observed that the biomass remained nearly constant, indicating little or no endogenous decay.

In the computer simulations, a comparison between the theoretical prediction (which included an assumed endogenous respiration term, $k = 0.05 / \text{hr}$) and the experimental data, showed that the endogenous requirement of the Pseudomonas putida could not account for the discrepancy in the data.

VIII. Conclusions and Recommendations

A. Conclusions

- * An existing mathematical model has been modified and verified with an inhibitory substrate.
- * It was experimentally verified that if an inhibitory waste is to be treated, there are cases where proper start-up of the unit (biomass concentration) is important for survival of the culture.
- * Quantitative discrepancies between predicted and calculated biomass concentration are most probably due to attachment of cells to the walls of the reactor.

B. Recommendations

As mentioned previously, the model needs to be extended to account for the wall attachment.

Although the mathematical model has been verified experimentally and the operating diagram has been generated, this was accomplished at zero initial phenol concentration in the reactor (i.e. $u = 0$).

It would be of interest to change the u_0 value and to get a different transient behavior.

In addition, although testing the model with a pure culture indicates that the modelling approach is correct, industrial applications generally involve the use of a mixed microbial population. In order to develop generalized methodologies to model mixed populations, it is necessary to characterize such populations, and determine the kinetic rate parameters for the dominant species. Various methodologies can then be employed to account for microbial interactions in the mixed culture.

Finally, the model should be extended to mixed substrates. If both mixed substrates and mixed species are employed in the reactor simultaneously, the modelling can become quite complex. However, this type of effort, in which the reactor design is approached from a more fundamental point of view, will ultimately produce much greater dividends in terms of cost-effective treatment of hazardous wastes.

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Table 1
PHENOL DEFINED MEDIUM SOLUTION [22]

Phenol	1000	mg
Ammonium Sulfate	500	mg
Magnesium Sulfate	100	mg
Ferric Chloride	0.5	mg
Manganese Sulfate	10	mg
1.0 M Potassium Phosphate Buffer Solution (pH 7.2)	30	ml
Tap Water	100	ml
Distilled Water	to volume of 1 liter	

Table 2

OPTICAL DENSITY vs TIME
(Pseudomonas Putida , ATCC 31800)

OPTICAL DENSITY , UOD
(at different initial phenol concentration , ppm)

Time (hr)	20	60	100	140	180	220
RUN 1						
0	0.006	0.008	0.005	0.010	0.009	0.006
0.5		0.011				
0.67	0.007					
1.0	0.008	0.014	0.008	0.013	0.011	
1.33	0.009	0.015				
1.67	0.010	0.017				
2.0	0.012	0.020	0.011	0.018	0.014	
2.33	0.014					
2.5		0.026				
3.0		0.034	0.015	0.025	0.019	
3.17		0.039				
3.67		0.049				
4.0			0.024	0.038	0.027	0.016
5			0.037	0.054	0.038	
6			0.056	0.072	0.050	
7					0.070	0.030
8					0.100	0.040
9						0.050
10						0.069
11						0.100

Table 2 continued

OPTICAL DENSITY , UOD (at different initial phenol concentration , ppm)						
Time (hr)	20	60	100	140	180	220
RUN 2						
0	0.006	0.006	0.006	0.009	0.010	0.008
0.33	0.007					
0.67	0.008	0.008				
1.0	0.009		0.009	0.015	0.012	
1.17		0.011				
1.33	0.010					
1.67	0.012	0.013				
2.0	0.013	0.015	0.012	0.017	0.014	
2.33	0.015	0.017				
2.83		0.019				
3.0			0.017	0.029	0.020	
3.17		0.023				
3.67		0.035				
4.0			0.027	0.041	0.030	0.022
4.17		0.052				
5.0			0.045	0.056	0.039	
6.0			0.068	0.070	0.048	
7.0					0.075	0.035
8.0					0.110	0.045
9.0						0.059
10.0						0.081
11.0						0.120

Table 2 continued

Time (hr)	OPTICAL DENSITY , UOD (at different initial phenol concentration ,ppm)					
	20	60	100	140	180	220
	RUN 3					
0	0.006	0.007	0.007	0.010	0.009	0.008
0.33	0.007					
0.67	0.008					
0.83		0.010				
1.0	0.009		0.010	0.012	0.012	
1.33	0.010	0.013				
1.67	0.011	0.015				
2.0	0.013	0.017	0.014	0.018	0.015	
2.33	0.015	0.019				
2.83		0.022				
3.0			0.020	0.026	0.021	
3.17		0.027				
3.67		0.040				
4.0			0.031	0.042	0.032	0.026
4.17		0.052				
5.0			0.050	0.054	0.040	
6.0			0.075	0.075	0.051	
7.0					0.068	0.049
8.0					0.095	0.058
9.0						0.072
10.0						0.095
11.0						0.013

Table 3

BIOMASS CONCENTRATION vs. TIME
(Pseudomonas Putida , ATCC 31800)

BIOMASS CONCENTRATION ppm (at different initial phenol concentration , ppm)						
Time (hr)	20	60	100	140	180	220
RUN 1						
0	1.57	2.07	1.30	2.59	2.33	1.56
0.5		2.85				
0.67	1.82					
1.0	2.07	3.64	2.07	3.37	2.85	
1.33	2.33	3.89				
1.67	2.59	4.41				
2.0	3.11	5.18	2.85	4.67	3.63	
2.33	3.63					
2.5		6.74				
3.0		8.78	3.89	6.48	4.93	
3.17		10.12				
3.67		12.71				
4.0			6.22	9.85	7.00	4.15
5			9.59	14.00	9.85	
6			14.52	18.66	12.96	
7					18.14	7.78
8					25.92	10.37
9						12.96
10						17.89
11						25.92

Table 3 continued

BIOMASS CONCENTRATION , ppm (at different initial phenol concentration , ppm)						
Time (hr)	20	60	100	140	180	220
RUN 2						
0	1.56	1.56	1.56	2.33	2.59	2.07
0.33	1.81					
0.67	2.07	2.07				
1.0	2.33		2.33	3.89	3.11	
1.17		2.85				
1.33	2.59					
1.67	3.11	3.37				
2.0	3.37	3.89	3.11	4.41	3.63	
2.33	3.89	4.41				
2.83		4.93				
3.0			4.41	7.52	5.18	
3.17		5.96				
3.67		9.07				
4.0			7.00	10.63	7.78	5.70
4.17		13.35				
5.0			11.66	14.52	10.11	
6.0			17.63	18.14	12.44	
7.0					19.44	9.07
8.0					28.51	11.66
9.0						15.29
10.0						21.00
11.0						31.10

Table 3 continued

BIOMASS CONCENTRATION , ppm (at different initial phenol concentration ,ppm)						
Time (hr)	20	60	100	140	180	220
RUN 3						
0	1.56	1.81	1.81	2.59	2.33	2.07
0.33	1.81					
0.67	2.07					
0.83		2.59				
1.0	2.33		2.59	3.11	3.11	
1.33	2.59	3.40				
1.67	2.85	3.89				
2.0	3.37	4.41	3.63	4.67	3.89	
2.33	3.89	4.93				
2.83		5.70				
3.0			5.18	6.74	5.44	
3.17		7.00				
3.67		10.37				
4.0			8.04	10.89	8.29	6.74
4.17		13.48				
5.0			12.96	14.00	10.37	
6.0			19.44	19.44	13.22	
7.0					17.63	12.70
8.0					24.62	15.03
9.0						18.66
10.0						24.62
11.0						33.70

Table 4

SUBSTRATE CONCENTRATION vs. TIME
(Pseudomonas Putida , ATCC 31800)

Time (hr)	SUBSTRATE CONCENTRATION ppm (at different initial phenol concentration , ppm)					
	20	60	100	140	180	220
	RUN 1					
0	19.2	57.5	100.4	137.3	178.0	219.3
0.5		54.2				
0.67	18.0					
1.0	16.8	51.3	98.1	134.1	176.4	
1.33	15.5	50.7				
1.67	14.0	49.1				
2.0	11.9	45.3	94.3	131.5	174.9	
2.33	10.2					
2.5		37.6				
3.0		30.0	91.6	125.9	170.5	
3.17		25.1				
3.67		14.0				
4.0			84.1	116.2	165.1	208.4
5			73.8	102.8	152.3	
6			55.9	86.4	143.4	
7					126.8	199.9
8					102.1	193.8
9						182.7
10						167.2
11						143.1

Table 4 continued

Time (hr)	SUBSTRATE CONCENTRATION , ppm (at different initial phenol concentration , ppm)					
	20	60	100	140	180	220
	RUN 2					
0	18.9	57.6	98.9	138.2	176.8	218.0
0.33	17.9					
0.67	16.7	54.3				
1.0	15.5		96.1	133.9	175.6	
1.17		52.7				
1.33	14.3					
1.67	12.0	50.9				
2.0	10.8	48.8	94.5	132.1	172.1	
2.33	9.2	46.9				
2.83		45.1				
3.0			90.7	124.8	168.9	
3.17		40.2				
3.67		25.8				
4.0			80.3	111.1	160.6	206.8
4.17		11.7				
5.0			67.2	99.2	149.6	
6.0			43.7	89.6	140.1	
7.0					119.8	198.9
8.0					89.2	192.6
9.0						179.3
10.0						158.9
11.0						130.4

Table 4 continued

Time (hr)	SUBSTRATE CONCENTRATION , ppm (at different initial phenol concentration , ppm)					
	20	60	100	140	180	220
RUN 3						
0	18.8	56.8	99.1	137.9	176.1	219.1
0.33	17.7					
0.67	16.4					
0.83		54.0				
1.0	15.4		96.4	136.5	174.5	
1.33	14.0	51.4				
1.67	12.9	49.1				
2.0	10.6	46.6	94.3	132.3	172.6	
2.33	8.7	45.7				
2.83		43.6				
3.0			88.5	125.8	166.1	
3.17		36.9				
3.67		22.3				
4.0			76.7	114.7	155.3	205.4
4.17		10.7				
5.0			64.1	101.7	150.8	
6.0			41.9	86.2	135.8	
7.0					127.1	189.4
8.0					105.1	180.1
9.0						167.5
10.0						145.6
11.0						117.2

Table 5
SPECIFIC GROWTH RATE vs.
INITIAL PHENOL CONCENTRATIONS FOR
Pseudomonas Putida (ATCC 31800)

Phenol Conc. (ppm)	SPECIFIC GROWTH RATE (1/hr)		
	RUN 1	RUN 2	RUN 3
20	0.367	0.373	0.378
60	0.472	0.480	0.465
100	0.396	0.398	0.404
140	0.346	0.345	0.353
180	0.307	0.304	0.295
220	0.247	0.238	0.243

Table 6
YIELD COEFFICIENT vs.
INITIAL PHENOL CONCENTRATIONS FOR
Pseudomonas Putida (ATCC 31800)

Phenol Conc. (ppm)	YIELD COEFFICIENT		
	RUN 1	RUN 2	RUN 3
20	0.223	0.232	0.226
60	0.243	0.251	0.248
100	0.301	0.293	0.308
140	0.320	0.315	0.322
180	0.306	0.294	0.305
220	0.321	0.325	0.305

Overall Average = 0.286 mg biomass/ mg substrate

Table 7
Andrews Parameters
For Pseudomonas Putida, ATCC 31800

k_i	:	51.000	ppm
k_s	:	47.101	ppm
μ	:	1.395	1/hr

Table 8

RESULTS OF RUN-SBR1
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies:

fill time	= 1 hr ;($\sigma_1=0.2$)
react time	= 3hrs , 53 min
draw time	= 7 min ;($\sigma_3=0.0233$)
total cycle time	= 5 hrs
phenol concentration in feed	= 35 ppm ;($u_f=0.7431$)
initial phenol concentration	= 0 ppm ;($u_0=0$)
initial biomass concentration	= 11.7 ppm ;($x_0=0.8659$)
initial reactor volume	= 2 liters
volume after fill phase	= 4 liters
volume after draw-down phase	= 2 liters ;($\delta=0.5$)
feed flow rate	= 2 lit/hr ;($\beta=13.95$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
1	22/9	22:00	11.7	0.0	6.91	7.13
		:20	9.1	8.6		
		:40	7.2	11.6		
		23:00	6.7	13.5		
		:20	7.2	11.4		
		:40	8.3	8.5		
	23/9	00:00	8.8	6.0	7.18	6.96
		:20	9.1	4.6		
		:40	10.1	3.0		
		01:00	10.1	2.3		
		:20	10.4	1.7		
		:40	10.6	1.3		
		02:00	10.6	0.8		
		:20	10.6	0.7		
1..2		:40	10.6	0.4	7.19	7.08
		03:00	10.9	0.3		

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
2		:20	8.3	8.8		
		:40	7.3	11.9		
		04:00	6.5	13.8	7.15	7.00
		:20	7.0	11.9		
		:40	7.8	9.0		
		05:00	8.3	6.7	7.19	6.92
		:20	8.8	5.2		
		:40	9.3	3.5		
		06:00	9.6	2.6	7.16	6.90
		:20	9.9	1.9		
		:40	9.9	1.5		
		07:00	9.9	1.3	7.18	6.87
		:20	10.1	0.8		
		:40	10.1	0.5		
2..3		08:00	10.4	0.4	7.18	7.04
3		:20	8.0	8.9		
		:40	7.0	12.1		
		09:00	6.7	14.0	7.17	6.95
		:20	7.3	12.1		
		:40	7.5	9.4		
		10:00	8.0	7.0	7.17	6.88
		:20	8.6	5.5		
		:40	9.3	4.1		
		11:00	9.3	2.8	7.20	6.83
		:20	9.6	2.0		
		:40	9.9	1.7		
		12:00	9.9	1.4	7.19	6.92
		:20	9.9	0.9		
		:40	10.1	0.6		
3..4		13:00	10.1	0.6	7.20	7.05

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)		
4		:20	7.8	9.1	7.18	6.96		
		:40	6.7	12.4				
		14:00	5.9	14.8				
		:20	6.5	12.6				
		:40	7.5	9.8				
		15:00	8.0	6.7			7.16	6.89
		:20	8.3	5.3				
		:40	9.1	4.1				
		16:00	9.1	3.1			7.19	6.81
		:20	9.3	2.2				
		:40	9.6	1.9				
		17:00	9.8	1.4			7.18	6.83
		:20	9.8	1.1				
		:40	9.8	0.7				
4..5		18:00	9.8	0.6	7.20	6.98		
8	24/9	09:20	7.4	8.1	7.18	7.02		
		:40	6.4	12.4				
		10:00	5.9	14.6				
		:20	6.4	12.3				
		:40	7.0	10.2				
		11:00	7.4	7.0			7.16	6.94
		:20	7.9	5.8				
		:40	8.3	4.7				
		12:00	8.8	3.1			7.19	6.89
		:20	8.8	2.3				
		:40	9.1	2.0				
		13:00	9.1	1.2			7.18	6.85
		:20	9.4	1.0				
		:40	9.4	0.7				
14:00	9.4	0.6	7.19	6.95				

Table 9

RESULTS OF RUN-SBR2
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies:

fill time	= 1 hr ;($\sigma_1=0.2$)
react time	= 3 hrs 53 min
draw-down time	= 7 min ;($\sigma_3=0.0233$)
total cycle time	= 5 hrs
phenol concentration in feed	= 100 ppm ;($u_f=2.1231$)
initial phenol concentration	= 0 ppm ;($u_0=0$)
initial biomass concentration	= 7.8 ppm ;($x_0=0.5772$)
initial reactor volume	= 2 liters
volume after fill phase	= 4 liters
volume after draw-down phase	= 2 liters ;($\delta=0.5$)
feed flow rate	= 2 lit/hr ;($\beta=13.95$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
1	28/9	23:00	7.8	0.0	6.89	7.26
		:30	5.2	31.8		
	29/9	00:00	4.4	46.1	7.09	7.14
		:30	6.5	40.2		
		01:00	8.6	32.5		
		:30	10.9	21.7		
		02:00	13.2	14.6		
		:30	15.8	7.4		
		03:00	17.1	3.1		
		:30	17.9	1.0		
1..2		04:00	18.4	0.5	7.11	7.16

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
2		:30	13.2	29.1		
		05:00	11.9	38.7	7.14	7.08
		:30	15.3	26.3		
		06:00	19.2	12.1	7.15	7.01
		:30	21.3	4.2		
		07:00	22.3	1.1	7.12	7.05
		:30	22.8	0.2		
		08:00	22.8	0.1	7.15	7.14
		:30	22.8	(0.03)		
2..3		09:00	22.8	(0.02)	7.14	7.17
3		:30	16.6	26.6		
		10:00	14.3	34.7	7.17	7.09
		:30	18.1	20.5		
		11:00	21.5	8.4	7.18	7.06
		:30	23.3	2.5		
		12:00	23.8	0.6	7.17	7.01
		:30	23.8	0.3		
		13:00	24.1	0.1	7.15	7.12
		:30	24.1	0.1		
3..4		14:00	24.1	0.0		
7	30/9	05:30	20.7	25.1		
		06:00	18.9	31.2	7.17	7.08
		:30	23.3	16.1		
		07:00	26.4	5.3	7.14	7.02
		:30	27.2	1.2		
		08:00	27.5	0.5	7.15	7.12
		:30	27.5	0.2		
		09:00	27.7	(0.04)	7.14	7.17
		:30	27.7	0.0		
7..8		10:00	28.0	0.0	7.15	7.16

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
8		:30	21.0	24.0		
		11:00	19.2	30.6	7.16	7.12
		:30	23.3	15.4		
		12:00	26.7	4.0	7.15	7.08
		:30	27.5	0.9		
		13:00	27.7	0.3	7.14	7.12
		:30	28.0	(0.02)		
		14:00	28.0	0.0	7.16	7.14
		:30	28.0	0.0		
		15:00	28.0	0.0	7.18	7.14

Table 10

RESULTS OF RUN-SBR3
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies

fill time	= 30 min ;($\sigma_1=0.4$)
react time	= 38 min
draw-down time	= 7 min ;($\sigma_3=0.093$)
total cycle time	= 1 hr 15 min
phenol concentration in feed	= 100 ppm ;($u_f=2.1231$)
initial phenol concentration	= 0 ppm ;($u_0=0$)
initial biomass concentration	= 15.6 ppm ;($x_0=1.1545$)
initial reactor volume	= 2 liters
volume after fill phase	= 4 liters
volume after draw-down phase	= 2 liters ;($\delta=0.5$)
feed flow rate	= 4 lit/hr ;($\beta=3.4875$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
1	30/9	22:00	15.6	0.0	6.97	7.28
		:15	10.9	30.8		
		:30	9.6	44.8		
		:45	10.4	40.2		
		23:00	11.7	35.1		
1..2		:15	12.7	32.5		
2	1/10	:30	9.3	51.5	7.20	7.01
		:45	8.0	60.4		
		00:00	8.8	56.9		
		:15	9.8	52.9		
		2..3		:30		

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO
3		:45	8.0	64.2		
		01:00	7.0	70.9	7.20	7.14
		:15	7.5	67.5		
		:30	8.6	63.6		
3..4		:45	9.5	61.8		
4		02:00	6.7	72.5	7.19	7.14
		:15	5.7	77.6		
		:30	6.2	74.6		
		:45	7.0	71.3		
4..5		03:00	7.8	69.9	7.18	7.10
10		10:45	2.1	92.7		
		11:00	1.8	93.9	7.21	7.18
		:15	2.1	93.2		
		:30	2.3	92.5		
10..11		:45	2.3	91.9		
11		12:00	1.8	94.1	7.20	7.16
		:15	1.3	95.1		
		:30	1.6	94.6		
		:45	1.8	94.0		
11..12		13:00	1.8	93.4	7.19	7.18
12		:15	1.3	95.3		
		:30	1.0	96.1		
		:45	1.3	95.7		
		14:00	1.3	95.2	7.20	7.18
12..13		:15	1.6	94.7		

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
18		20:45	0.5	98.9		
		21:00	0.5	99.1	7.24	7.20
		:15	0.5	99.0		
		:30	0.5	98.8		
18..19		:45	0.5	98.8		
19		22:00	0.5	99.1	7.22	7.19
		:15	0.3	99.3		
		:30	0.5	99.2		
		:45	0.5	99.1		
19..20		23:00	0.5	99.1	7.23	7.20
20		23:15	0.5	99.3		
		:30	0.3	99.5		
		:45	0.5	99.5		
	2/10	00:00	0.5	99.3	7.23	7.21
		:15	0.5	99.3		

Table 11

RESULTS OF RUN-SBR4
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies:

fill time : 1 hr ;($\sigma_1=0.2$)
 react time : 3 hr 53 min
 draw-down time : 7 min ;($\sigma_3=0.0233$)
 total cycle time : 5 hrs
 phenol concentration in feed : 100 ppm ;($u_f=2.1231$)
 initial phenol concentration : 0 ppm ;($u_0=0$)
 initial biomass concentration : 16.2 ppm ;($x_0=1.2$)
 initial reactor volume : 2 liters
 volume after fill phase : 4 liters
 volume after draw-down phase : 2 liters ;($\delta=0.5$)
 feed flow rate : 2 lit/hr ;($\beta=13.95$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)		
1	25/10	23:00	16.2	0.0	6.98	7.25		
		:30	12.2	28.5				
	26/10	00:00	11.1	38.4	7.18	7.04		
		:30	14.0	27.9				
		01:00	17.1	16.9				
		:30	20.7	8.9				
		02:00	21.5	2.5				
		:30	22.0	1.0				
		03:00	22.0	0.5			7.20	7.06
		:30	22.0	0.1				
1..2		04:00	22.0	(0.04)				

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)		
2		:30	17.1	26.4	7.14	7.16		
		05:00	15.6	34.0				
		:30	19.2	20.7				
		2..3		06:00	22.3	9.6	7.17	7.03
				:30	25.1	4.3		
				07:00	25.1	0.5		
				:30	25.4	0.1		
				08:00	25.4	0.1		
				:30	25.4	0.1		
				09:00	25.4	(0.02)		
3		:30	19.4	25.3	7.16	7.14		
		10:00	17.6	32.0				
		:30	21.5	17.7				
		3..4		11:00	24.6	7.2	7.18	7.04
				:30	26.4	3.3		
				12:00	27.0	0.2		
				:30	27.0	0.1		
				13:00	27.0	0.1		
				:30	27.0	0.1		
				14:00	27.0	0.0		
6	27/10	00:30	20.7	23.9	7.18	7.15		
		01:00	19.2	30.1				
		:30	23.3	14.7				
		6..7		02:00	26.2	4.2	7.17	7.07
				:30	27.2	1.3		
				03:00	27.5	0.4		
				:30	27.7	0.1		
				04:00	27.7	0.1		
				:30	27.7	0.0		
				05:00	27.7	0.0		

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
7		:30	21.0	23.8		
		06:00	19.4	29.9	7.15	7.17
		:30	23.6	14.5		
		07:00	26.2	4.1		
		:30	27.5	1.3		
		08:00	27.7	0.4	7.18	7.05
		:30	28.0	0.1		
		09:00	28.0	0.0		
		:30	28.0	0.0		
		10:00	28.0	0.0		

Table 12

RESULTS OF RUN-SBR5
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies:

fill time	= 30 min ;($\sigma_1=0.28$)
react time	= 1 hr 10 min
draw-down time	= 7 min ;($\sigma_3=0.065$)
total cycle time	= 1 hr 47 min
phenol concentration in feed	= 140 ppm ;($u_f=2.9723$)
initial phenol concentration	= 0 ppm ;($u_0=0$)
initial biomass concentration	= 16.2 ppm ;($x_0=1.2$)
initial reactor volume	= 2 liters
volume after fill phase	= 4 liters
volume after draw-down phase	= 2 liters ;($\delta=0.5$)
feed flow rate	= 4 lit/hr ;($\beta=5.0$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
1	28/10	21:00	16.2	0.0	6.94	7.09
		:15	10.9	44.1		
		:30	9.1	66.0		
		:45	10.6	60.5		
		22:00	12.2	53.5	7.08	6.82
		:15	14.0	47.5		
		:30	16.1	43.2		
		:45	17.6	36.7		
1..2						
2	29/10	23:02	12.2	67.5	7.10	7.02
		:17	10.1	83.3		
		:32	11.7	77.6		
		:47	13.2	70.4		
		00:02	15.3	64.1	7.14	6.91
		:17	17.4	59.4		
		:32	19.2	52.5		
		2..3				

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
10		13:18	23.6	61.4	7.10	7.04
		:33	18.4	75.5		
		:48	20.7	66.2		
		14.03	23.8	54.8		
		:18	27.0	43.6	7.12	6.87
		:33	30.6	33.9		
10..11		:48	33.2	23.7		
18	30/10	03:34	27.2	43.1	7.11	6.98
		:49	22.2	59.5		
		04:04	25.2	48.2		
		:19	28.8	33.1	7.13	6.71
		:34	32.1	20.9		
		:49	35.5	11.3		
		05:04	37.1	6.4		
19		05:21	27.2	43.1	7.12	6.99
		:36	22.0	59.7		
		:51	25.7	48.8		
		06:06	29.0	33.4	7.14	6.75
		:21	32.4	21.5		
		:36	35.5	11.0		
		:51	37.1	6.0		

table 13

RESULTS OF RUN-SBR6
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies :

fill time	= 30 min ;($\sigma_1=0.28$)
react time	= 1 hr 10 min
draw-down time	= 7 min ;($\sigma_3=0.065$)
total time	= 1 hr 47 min
phenol concentration in feed	= 140 ppm ;($u_f=2.9723$)
initial phenol concentration	= 0 ppm ;($u_0=0$)
initial biomass concentration	= 35.0 ppm ;($x_0=2.6$)
initial reactor volume	= 2 liters
volume after fill phase	= 4 liters
volume after draw-down phase	= 2 liters ;($\delta=0.5$)
feed flow rate	= 4 lit/hr ;($\beta=5$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)
1	3/11	23:00	35.0	0.0	7.02	7.14
		:15	24.1	40.2		
		:30	20.0	58.1		
		:45	23.1	49.0		
		4/11	00:00	26.7		
1..2		:15	29.8	22.3		
		:30	32.9	13.2		
		:45	34.7	7.1		
2		01:02	24.4	44.8	7.14	7.08
		:17	20.2	61.3		
		:32	23.3	52.2		
		:47	27.2	35.1		
		02:02	30.3	24.8		
2..3		:17	33.7	14.9		
		:32	35.5	8.2		

Cycle	Date	Time	Biomass Conc. (ppm)	Sybststrate Conc. (ppm)	pH	DO (ppm)		
5		06:23	25.9	43.7	7.13	7.04		
		:38	21.0	61.2				
		:53	24.4	50.0				
		5..6		07:08	28.5	33.1	7.18	6.90
				:23	31.9	22.3		
				:38	34.5	11.2		
				:53	36.8	6.2		
10		15:18	26.4	43.1	7.15	7.08		
		:33	21.3	60.7				
		:48	24.6	48.9				
		10..11		16:03	28.8	32.3	7.19	6.88
				:18	32.1	21.5		
				:33	34.5	10.6		
				:48	37.1	5.8		
11		17:05	26.4	43.0	7.16	7.07		
		:20	21.3	60.5				
		:35	24.9	49.1				
		11..12		:50	29.0	32.1	7.15	6.91
				18:05	32.4	21.2		
				:20	35.0	10.4		
				:35	37.3	5.6		

Table 14

RESULTS OF RUN-SBR7
(Pseudomonas Putida, ATCC 31800)

Experimental Strategies:

fill time	= 30 min ;($\sigma_1=0.28$)
react time	= 1 hr 10 min
draw-down time	= 7 min ;($\sigma_3=0.065$)
total cycle time	= 1 hr 47 min
phenol concentration in feed	= 140 ppm ;($u_f=2.9732$)
initial phenol concentration	= 0 ppm ;($u_0=0$)
initial biomass concentration	= 4.2 ppm ;($x_0=0.31$)
initial reactor volume	= 2 liters
volume after fill phase	= 4 liters
volume after draw-down phase	= 2 liters ;($\delta=0.5$)
feed flow rate	= 4 lit/hr ;($\beta=5$)

Cycle	Date	Time	Biomass Conc. (ppm)	Substrate Conc. (ppm)	pH	DO (ppm)		
1	25/11	23:00	4.2	0.0	6.98	7.11		
		:15	2.6	41.1				
		:30	2.3	67.4				
		:45	2.6	65.1				
		26/11 00:00	3.4	67.0			7.09	7.02
1..2		:15	3.9	62.3				
		:30	4.1	60.2				
		:45	4.9	59.1				
10		15:18	1.6	129.8	7.05	7.07		
		:33	1.0	131.0				
		:48	1.3	133.6				
		16:03	1.3	133.1				
		:18	1.6	132.7			7.08	6.99
		:33	1.8	132.1				
10..11		:48	2.1	131.4				
20	27/11	09:08	0.5	138.3	7.08	7.16		
		:23	0.3	138.8				
		:38	0.5	138.4				
		:53	0.5	138.1				
		10:08	0.5	137.8			7.11	7.14
		:23	0.5	137.8				
20..21		:38	0.5	137.5				

21	:55	0.5	138.5	7.10	7.15
	11:10	0.3	139.0		
	:25	0.5	138.6		
	:40	0.5	138.4		
	:55	0.5	138.0	7.13	7.14
	12:10	0.5	138.0		
	:25	0.5	137.9		

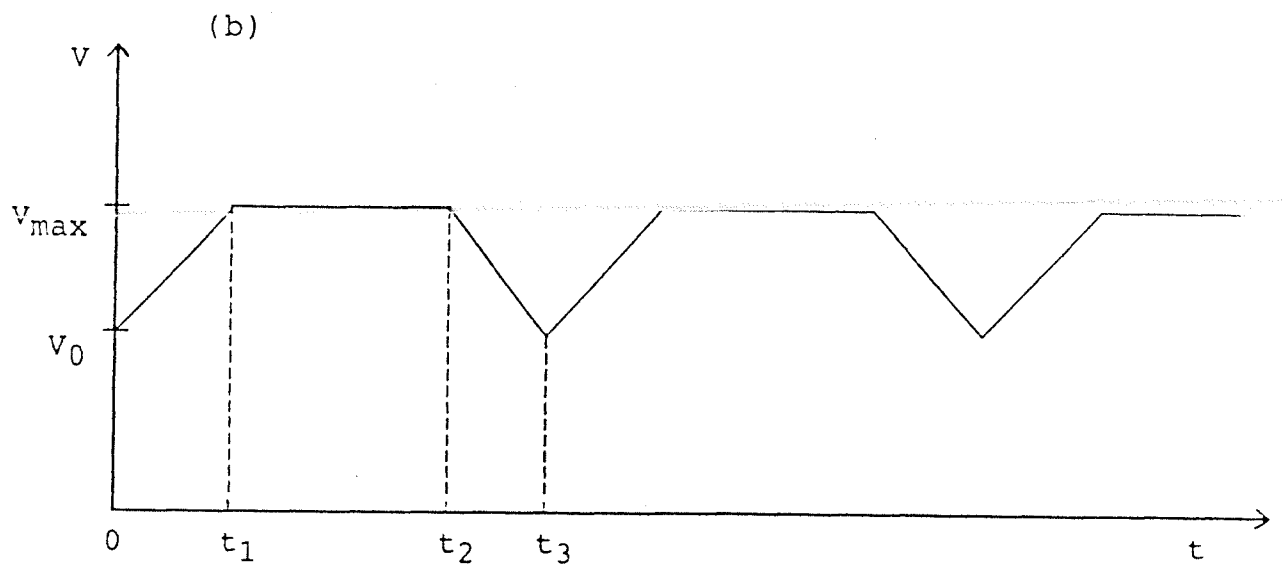
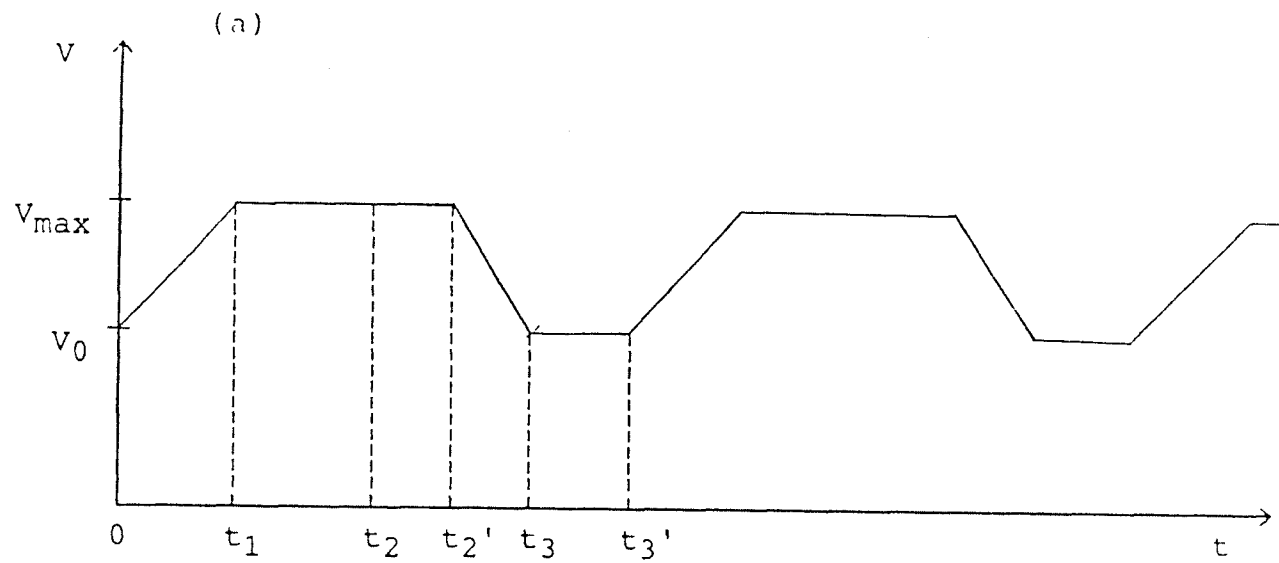
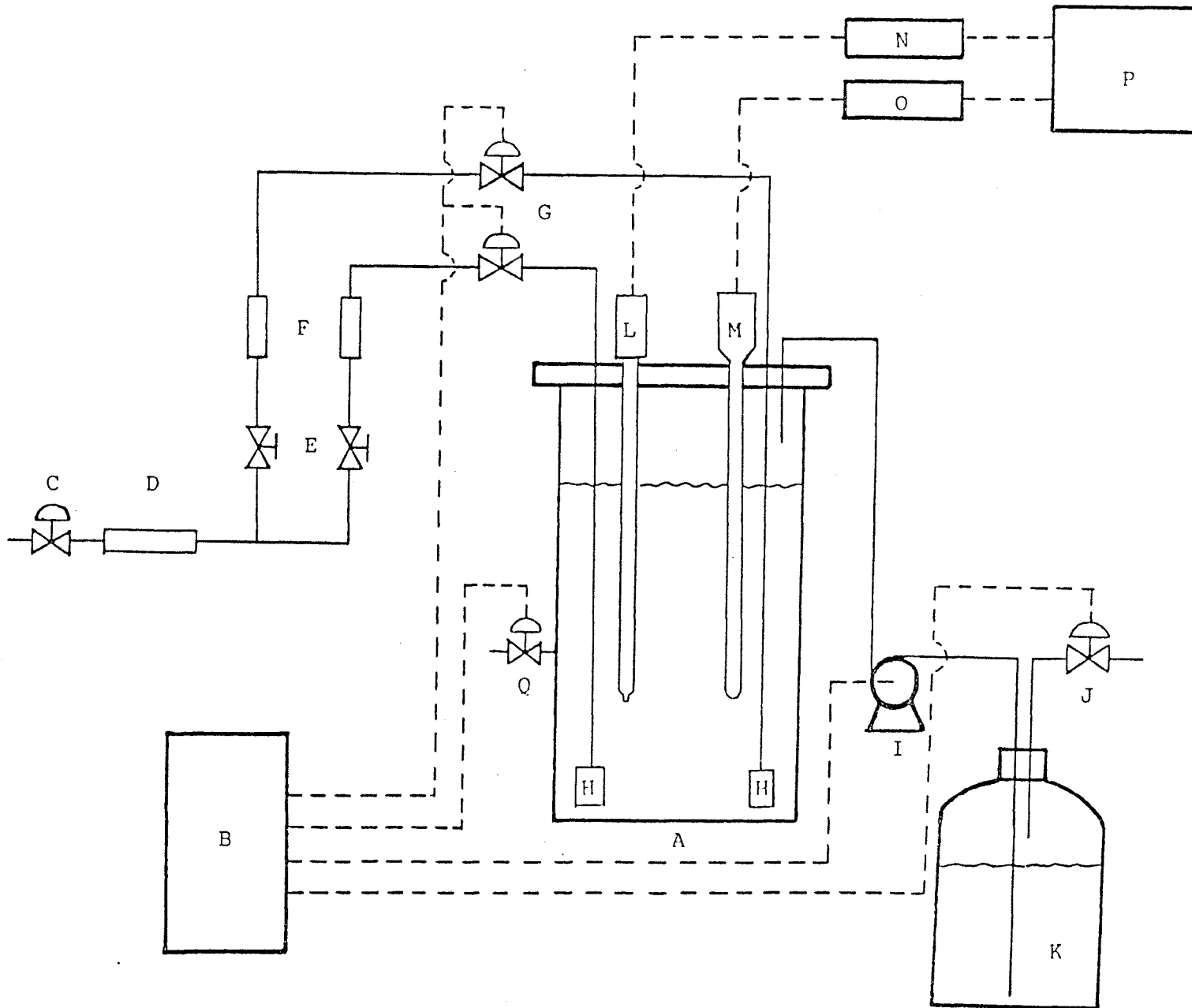
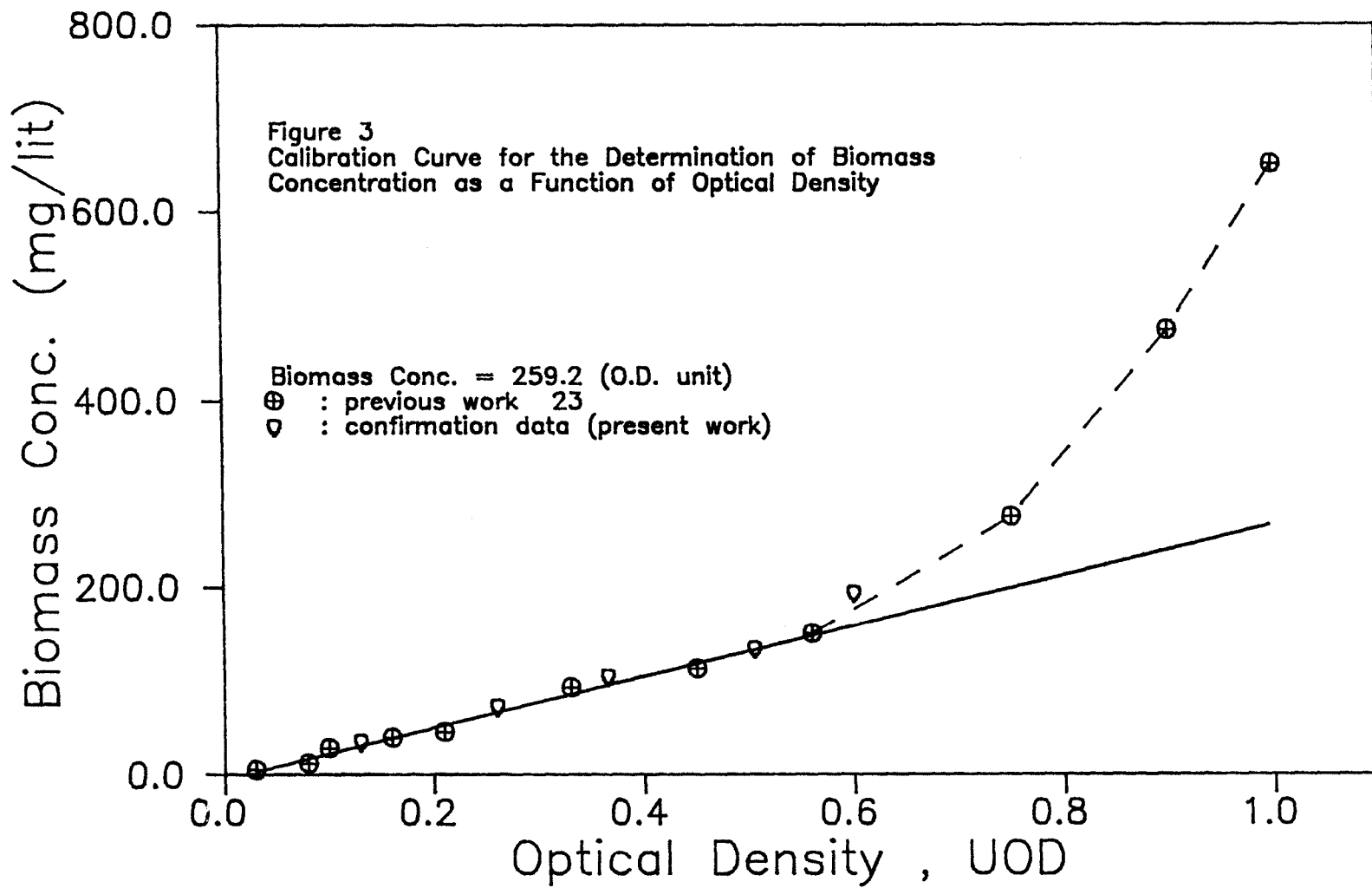


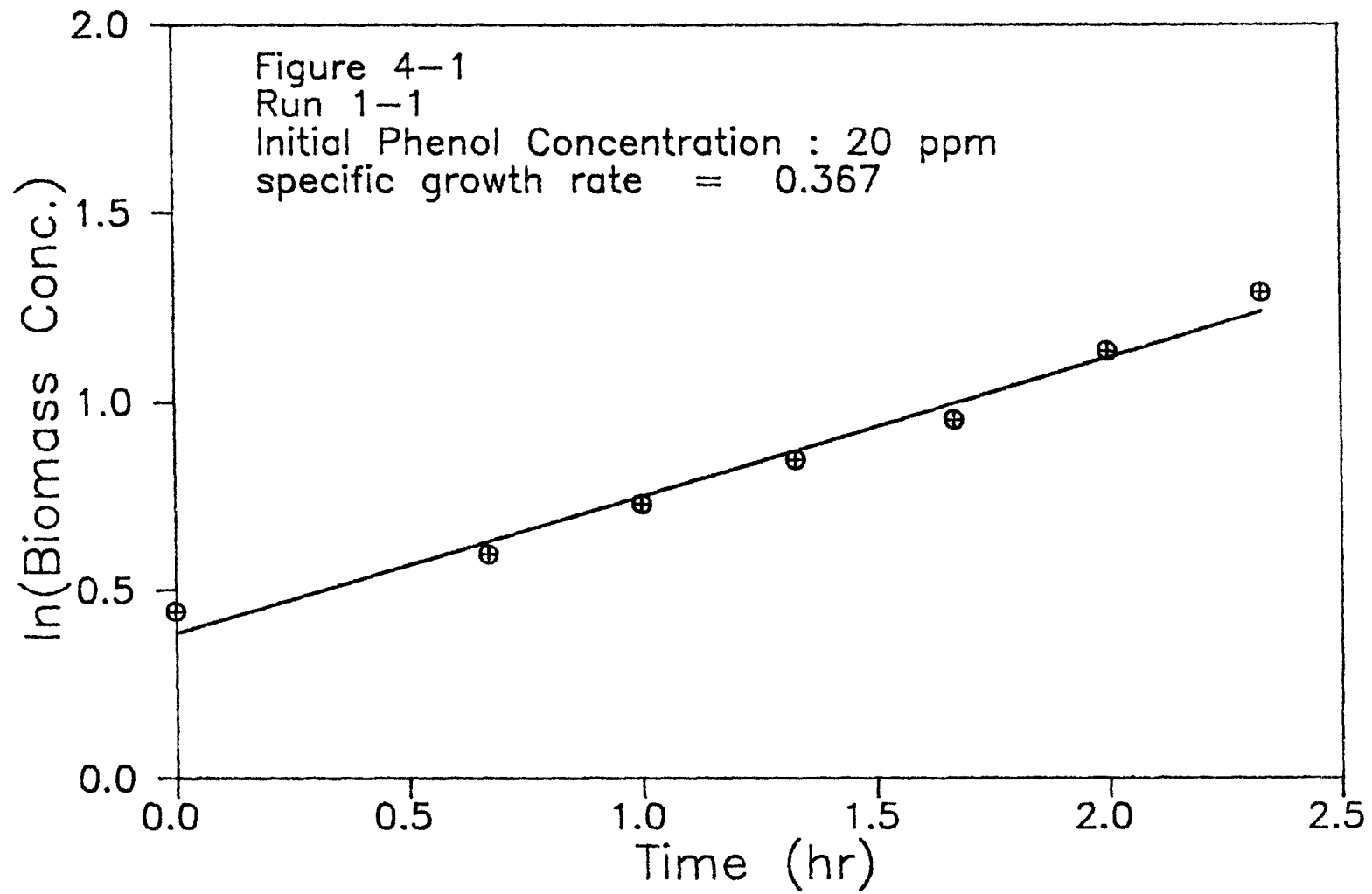
Figure 1 - Qualitative Representation of the Volume Change During Cycles: (a) generalized case; (b) special case (with no settle phase).

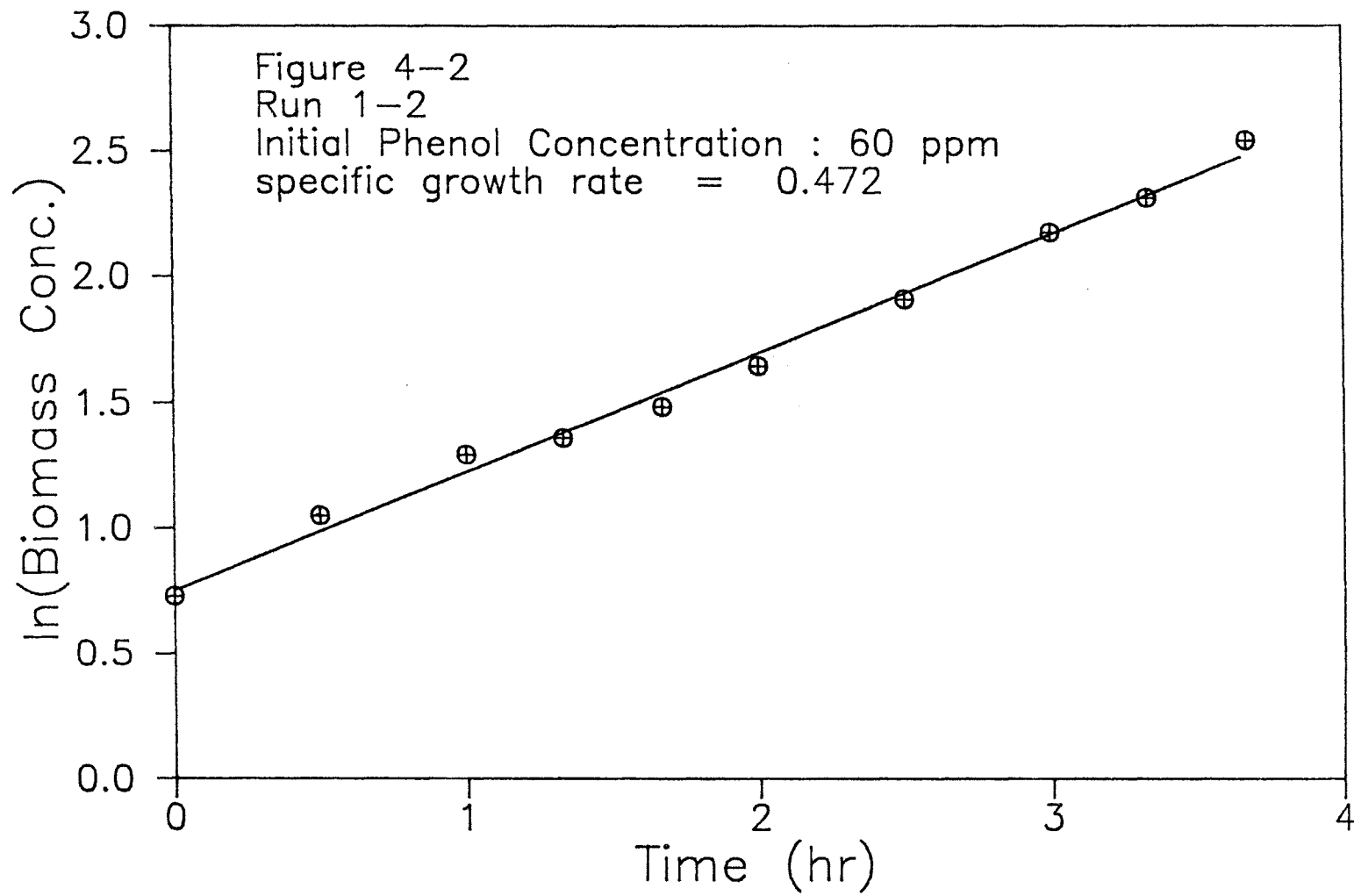


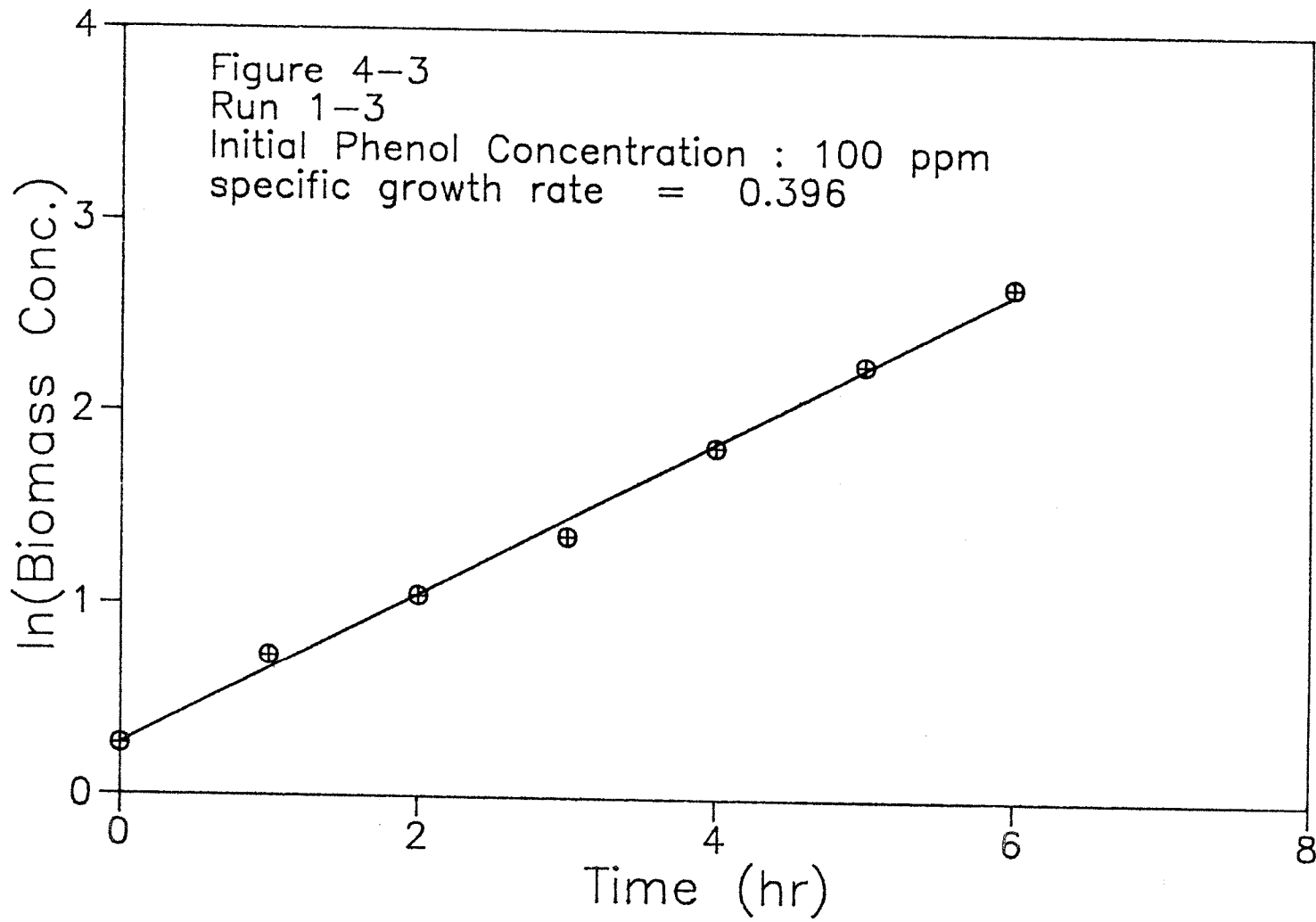
- A. Reactor
- B. Microprocessor
- C. Main Valve
- D. Air Filter
- E. Rotameter Control
- F. Rotameter
- G. Air Solenoid Valves
- H. Diffuser Stone
- I. Influent Pump
- J. Feed Solenoid Valve
- K. Feed Bottle
- L. pH Electrode
- M. D.O. Electrode
- N. pH Indicator
- O. D.O. Indicator
- P. Recorder
- Q. Decant Solenoid Valve

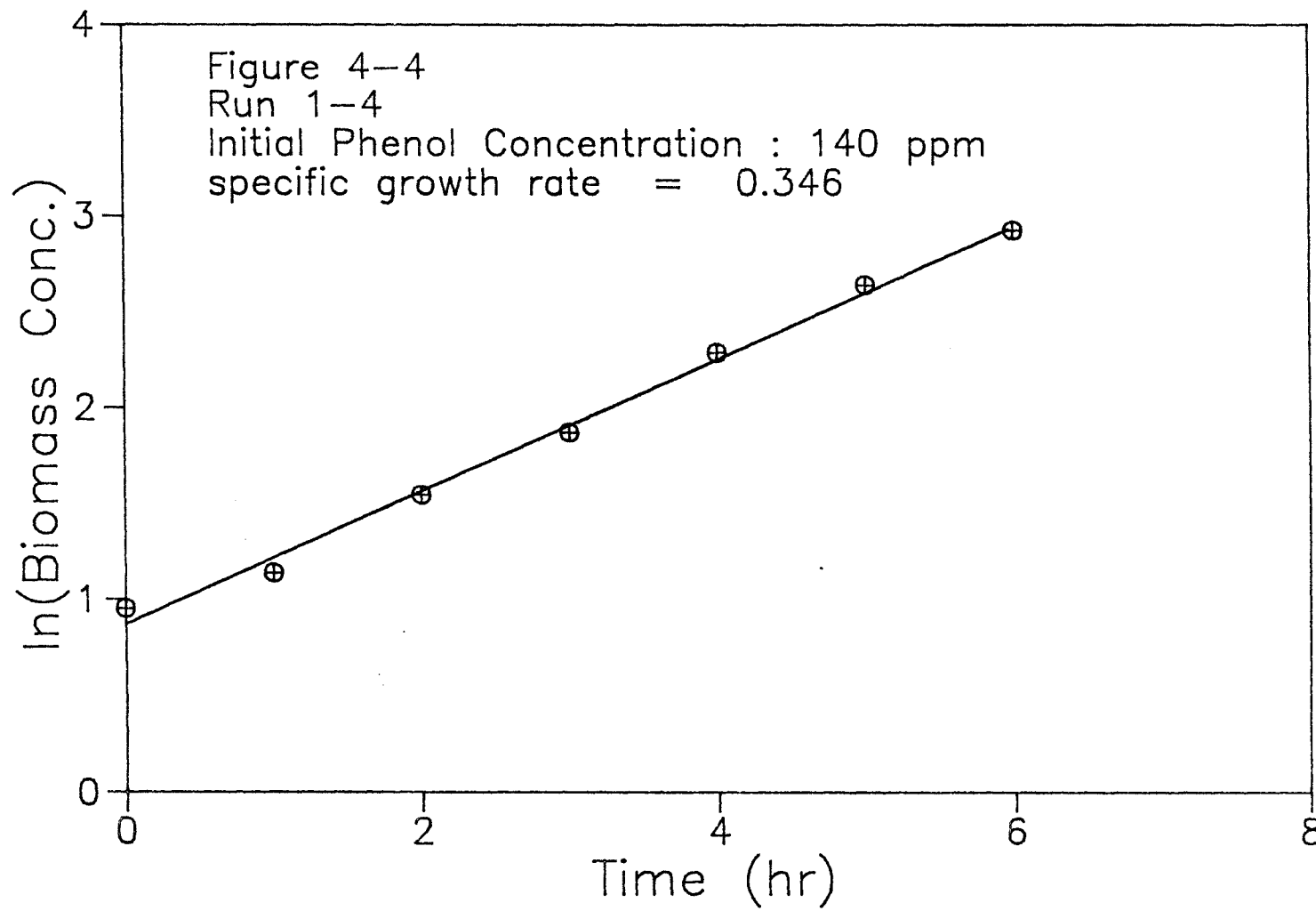
Figure 2 : Schematic diagram of Sequencing Batch Reactor

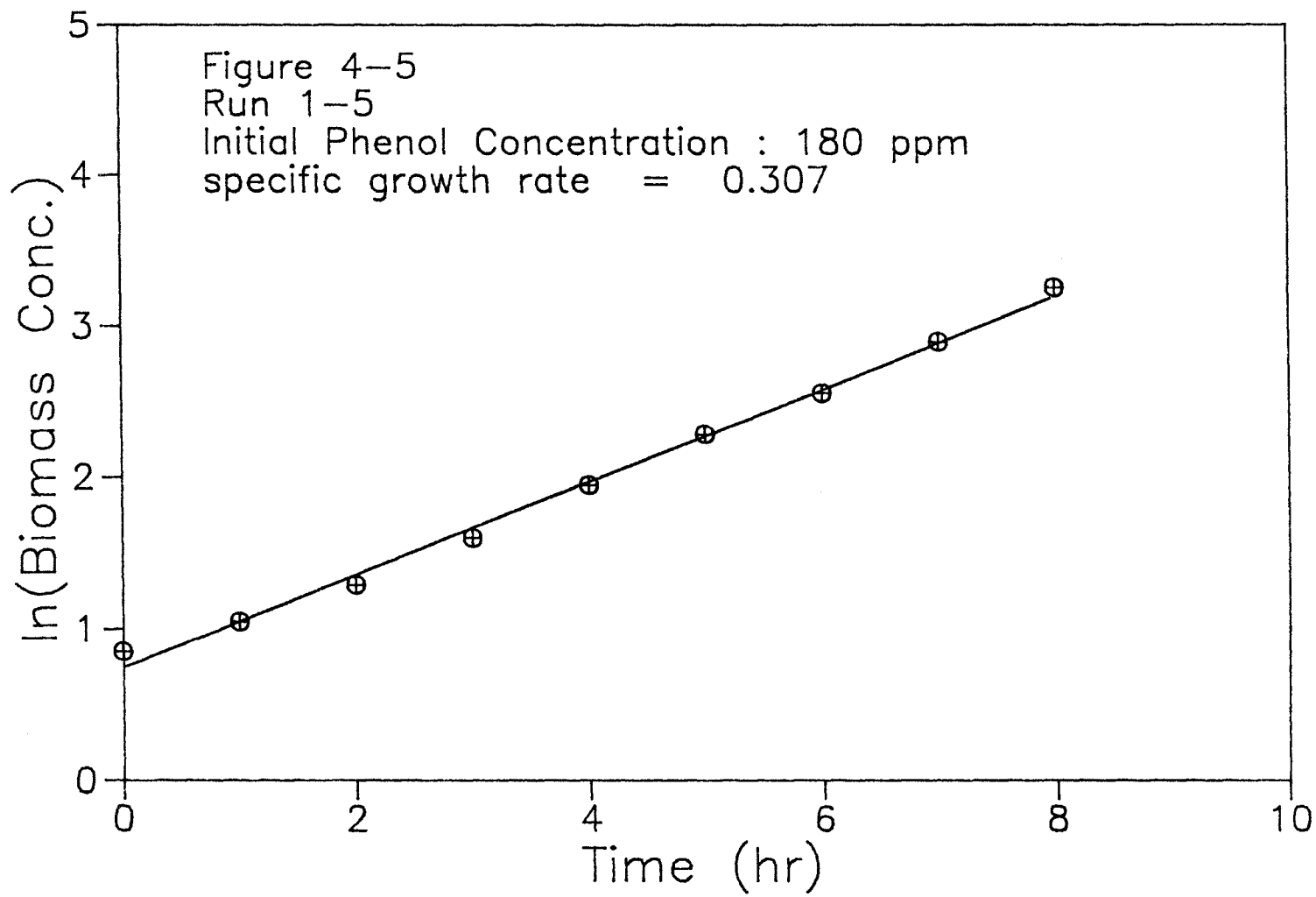


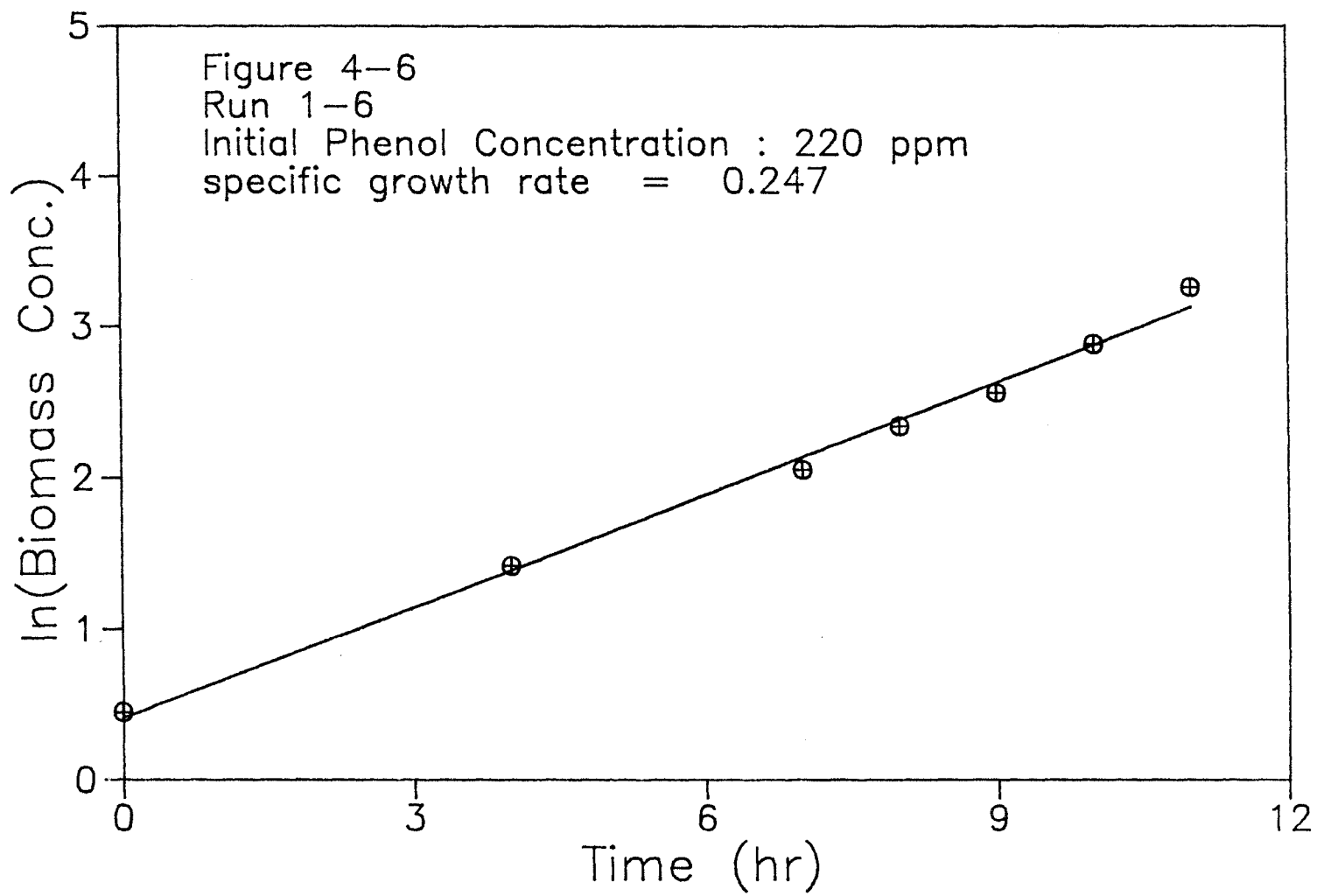


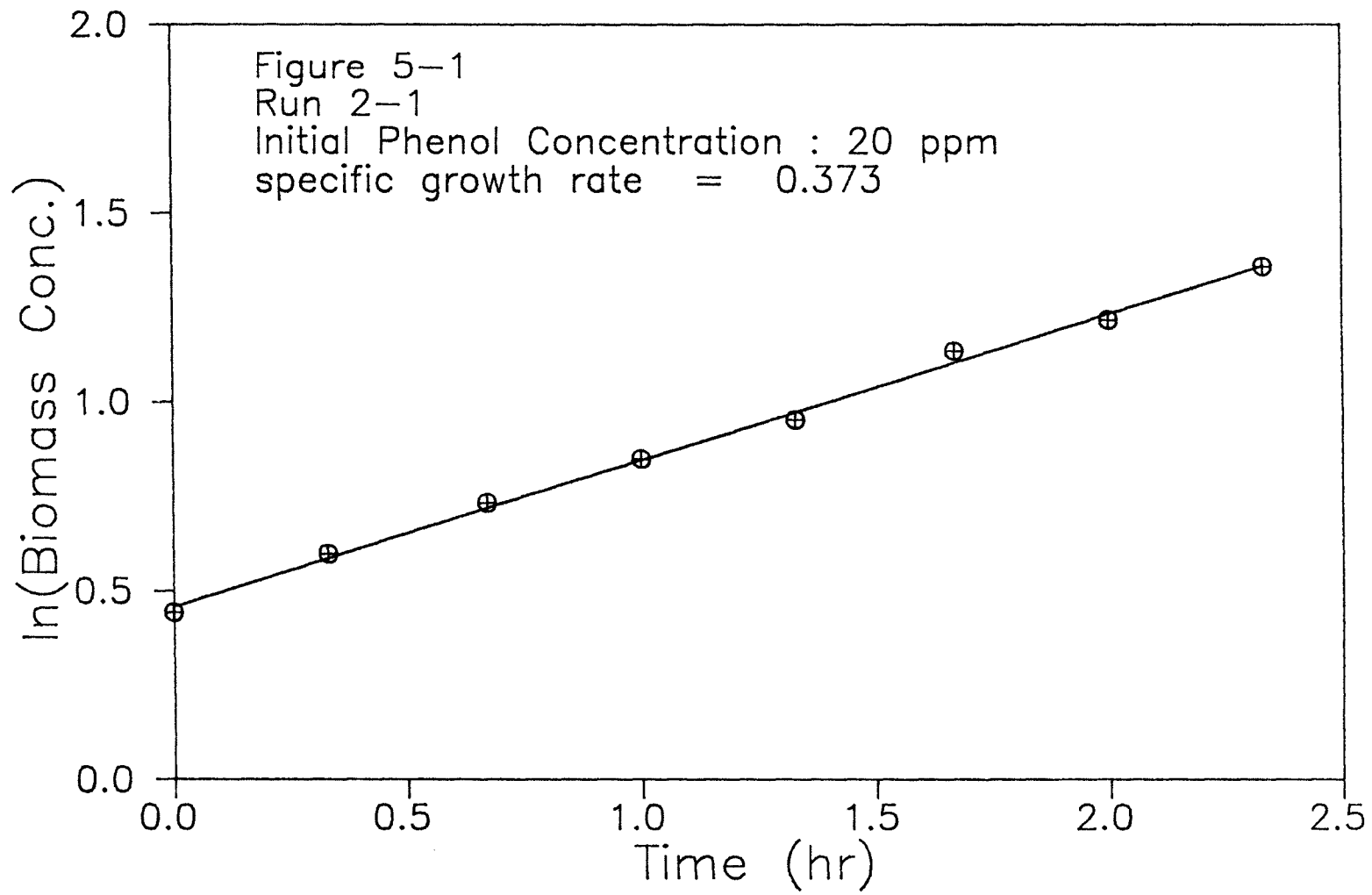


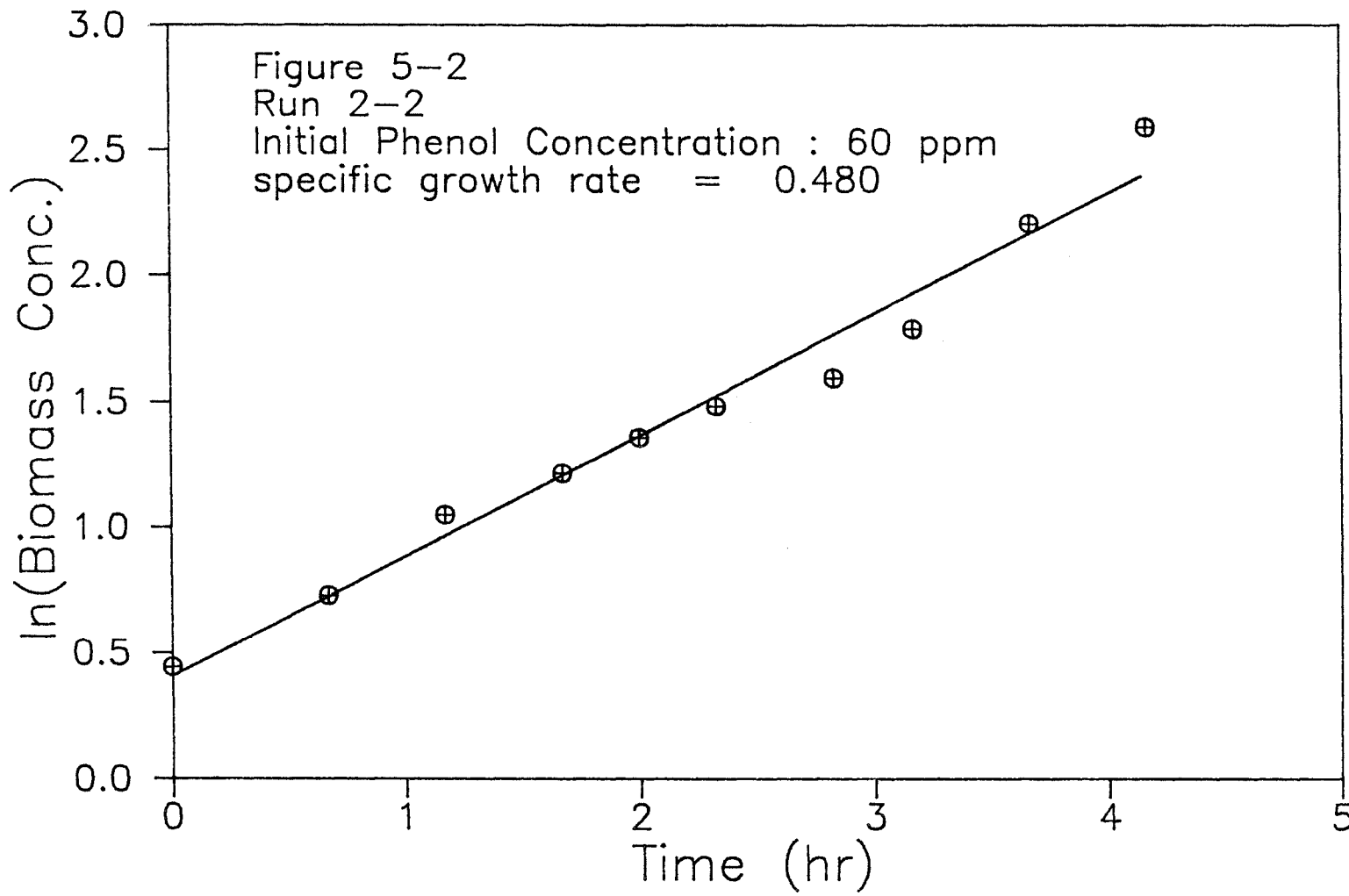


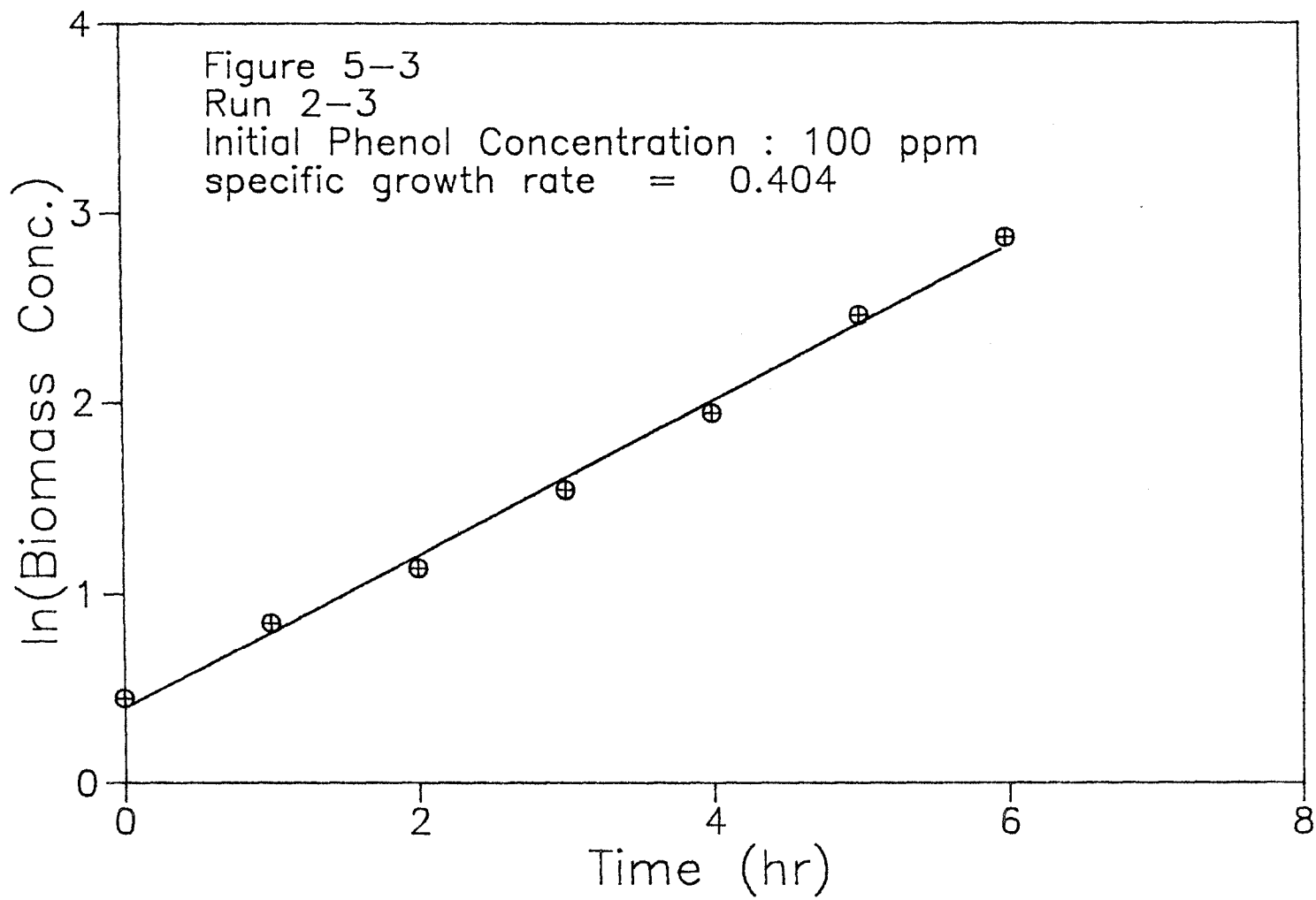


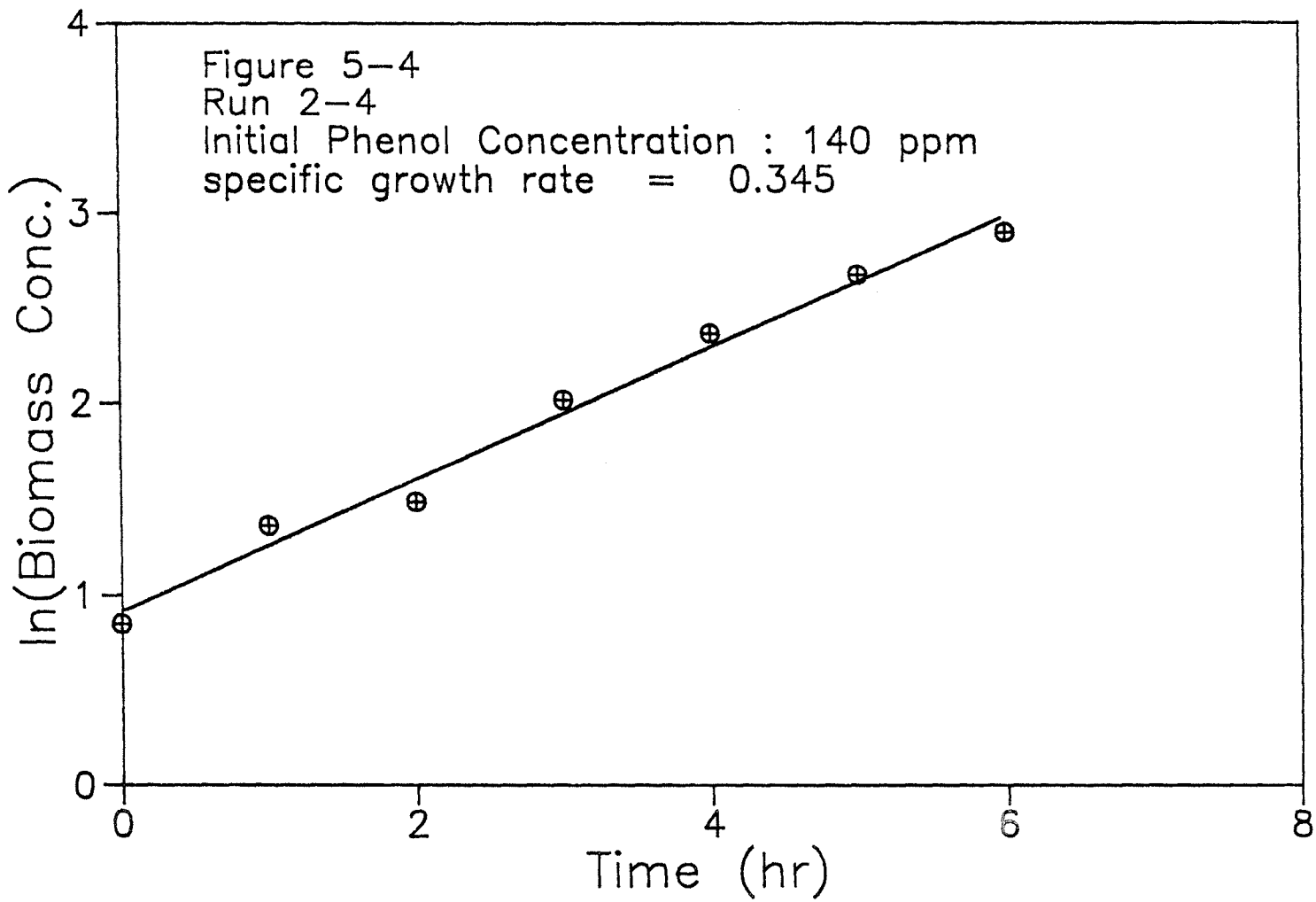


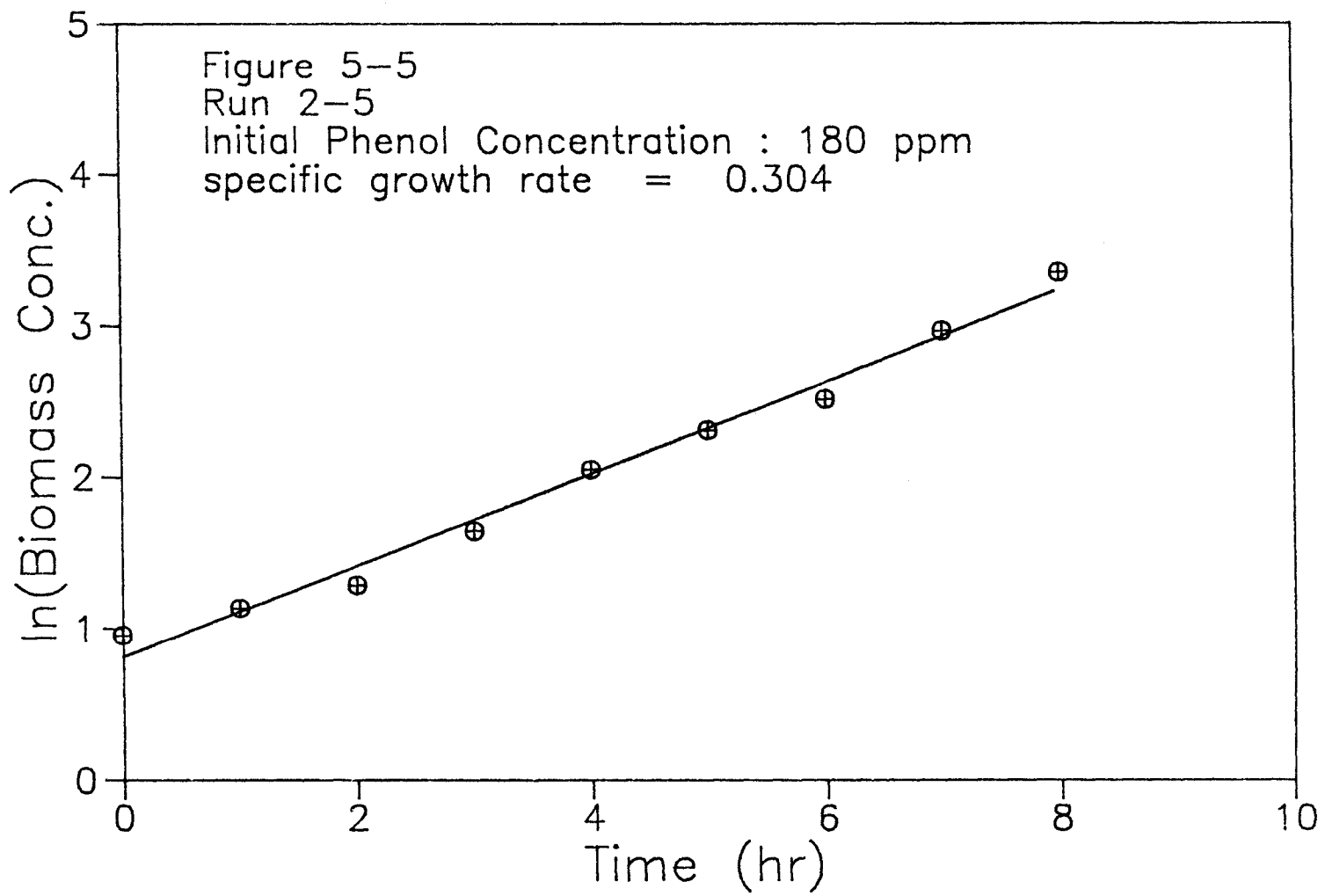


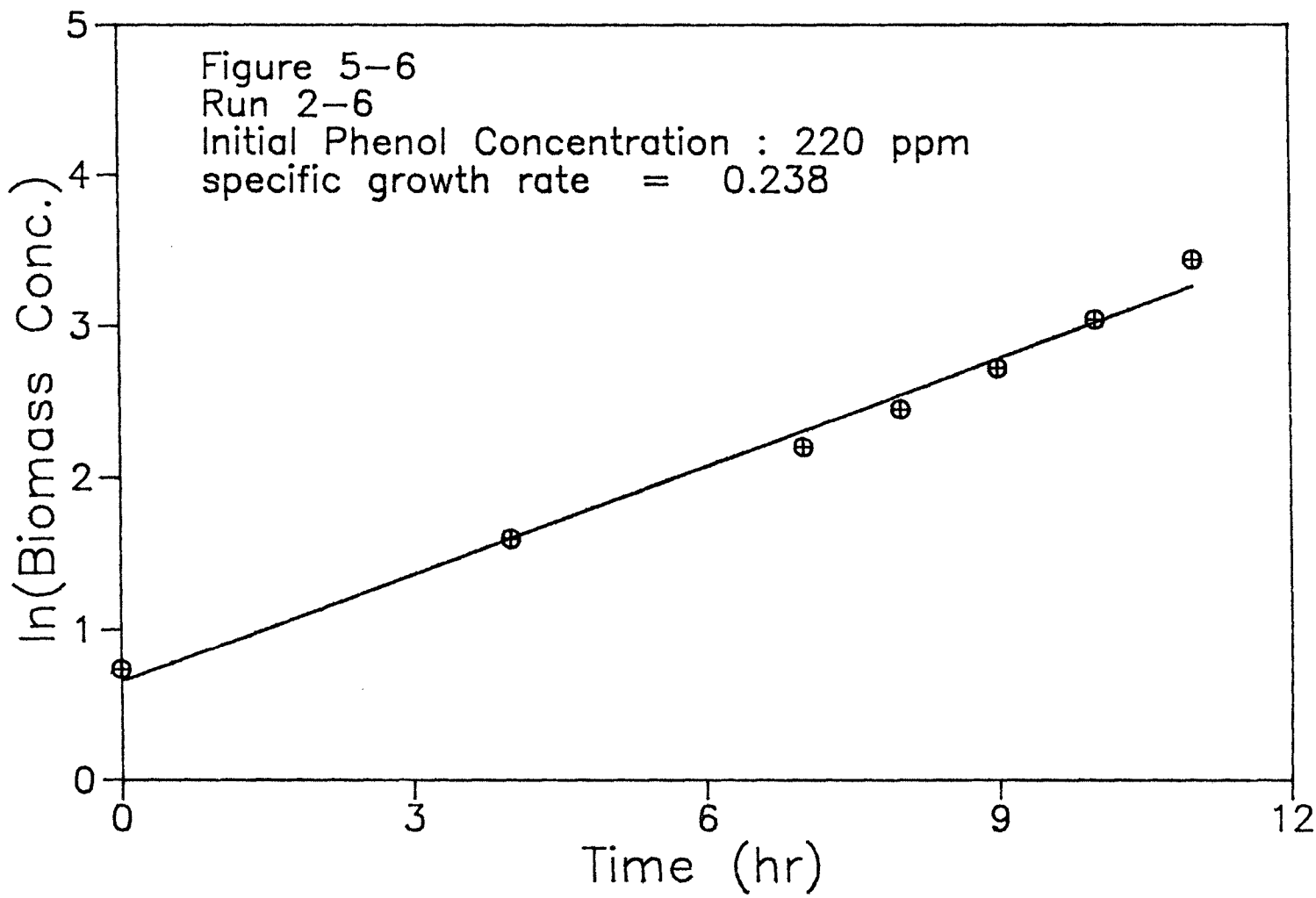


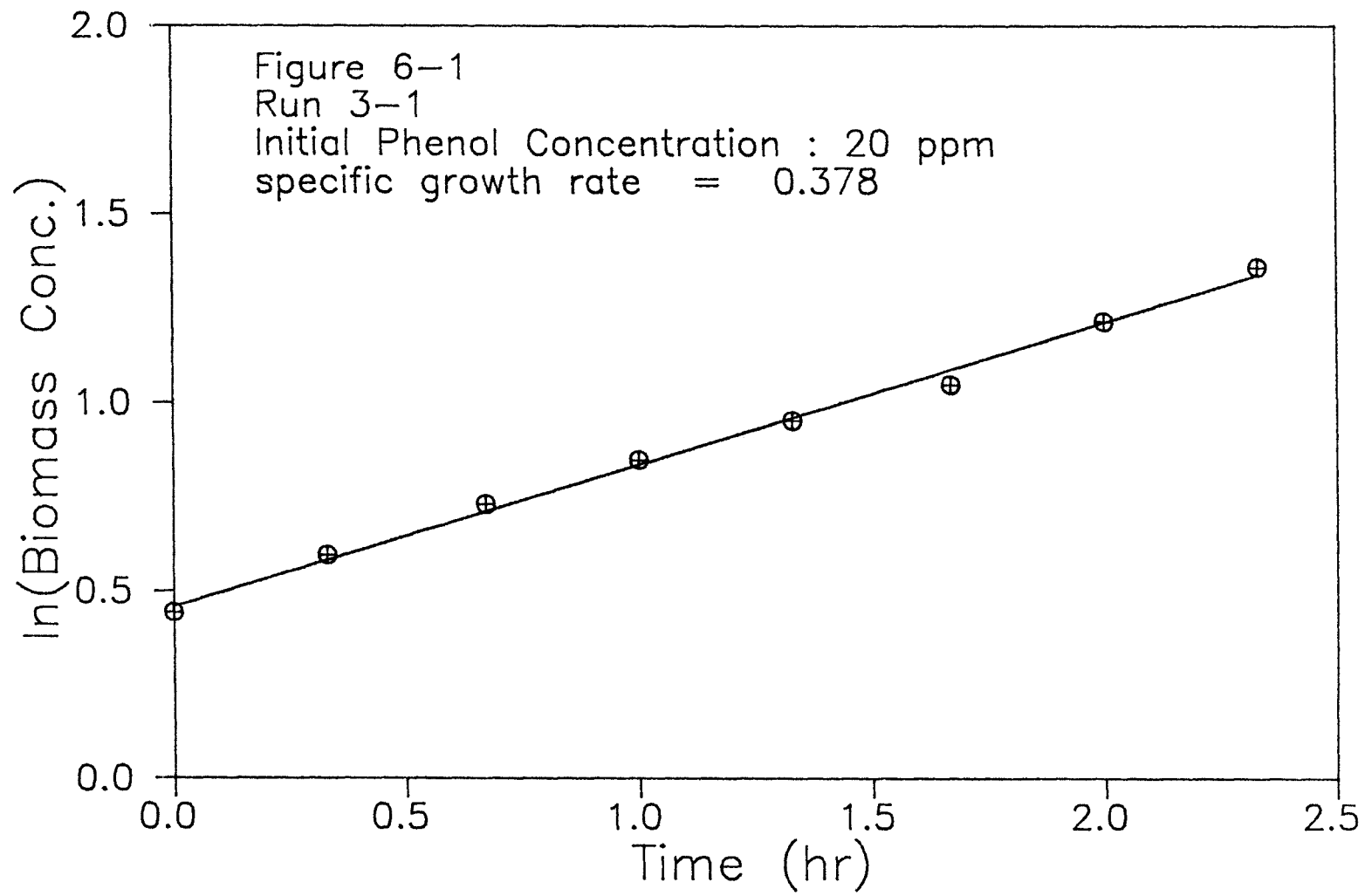


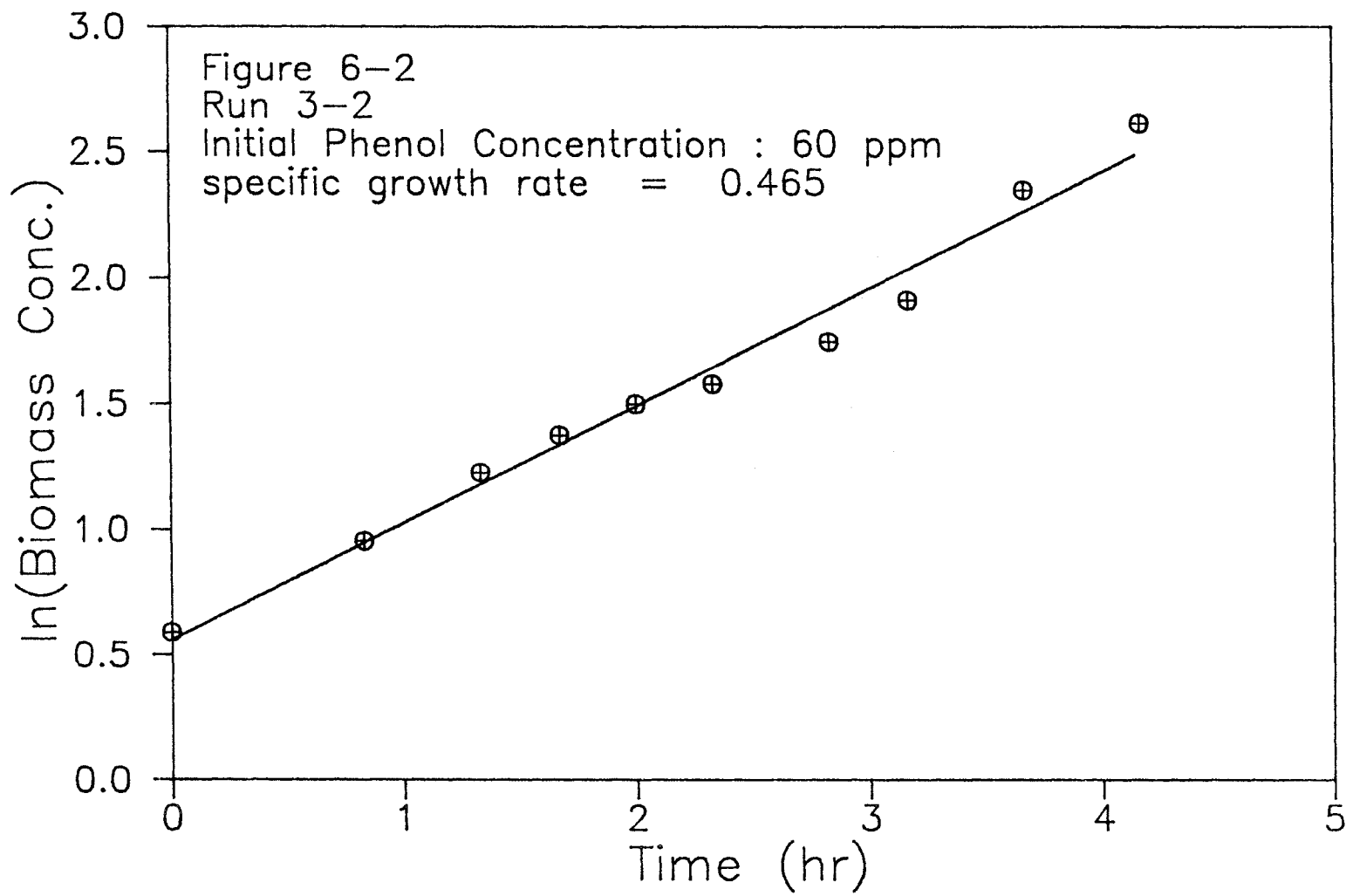


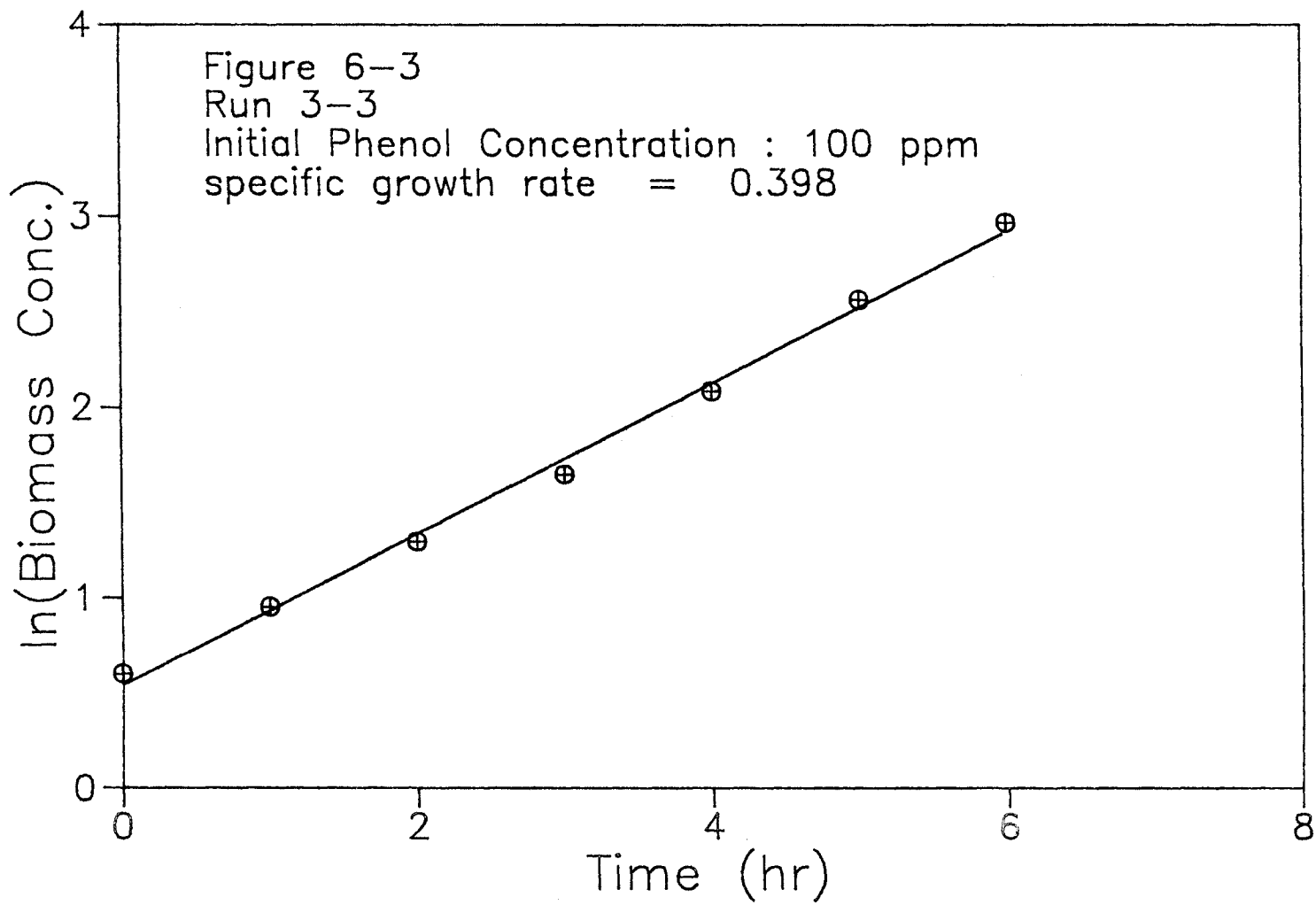


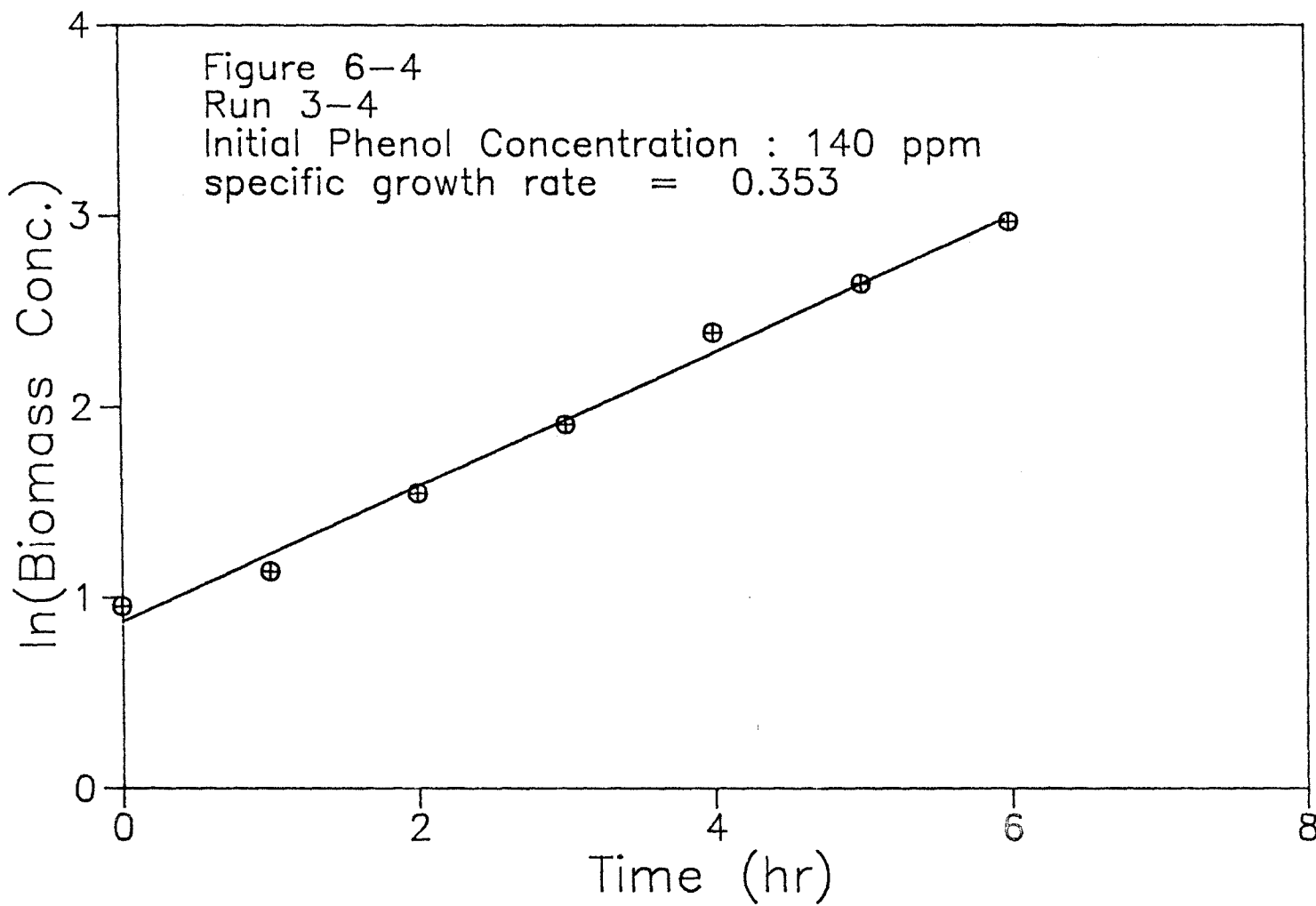


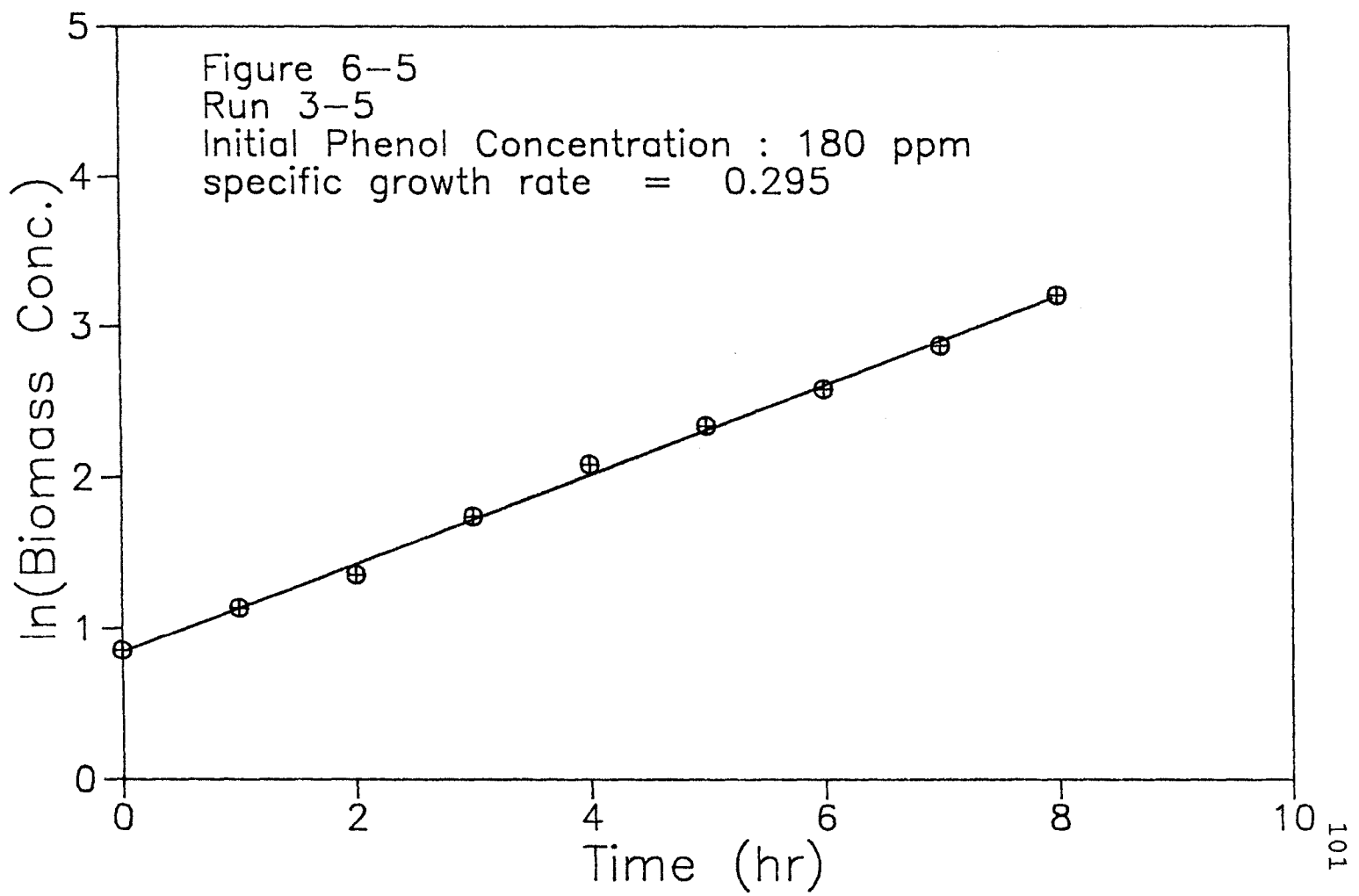


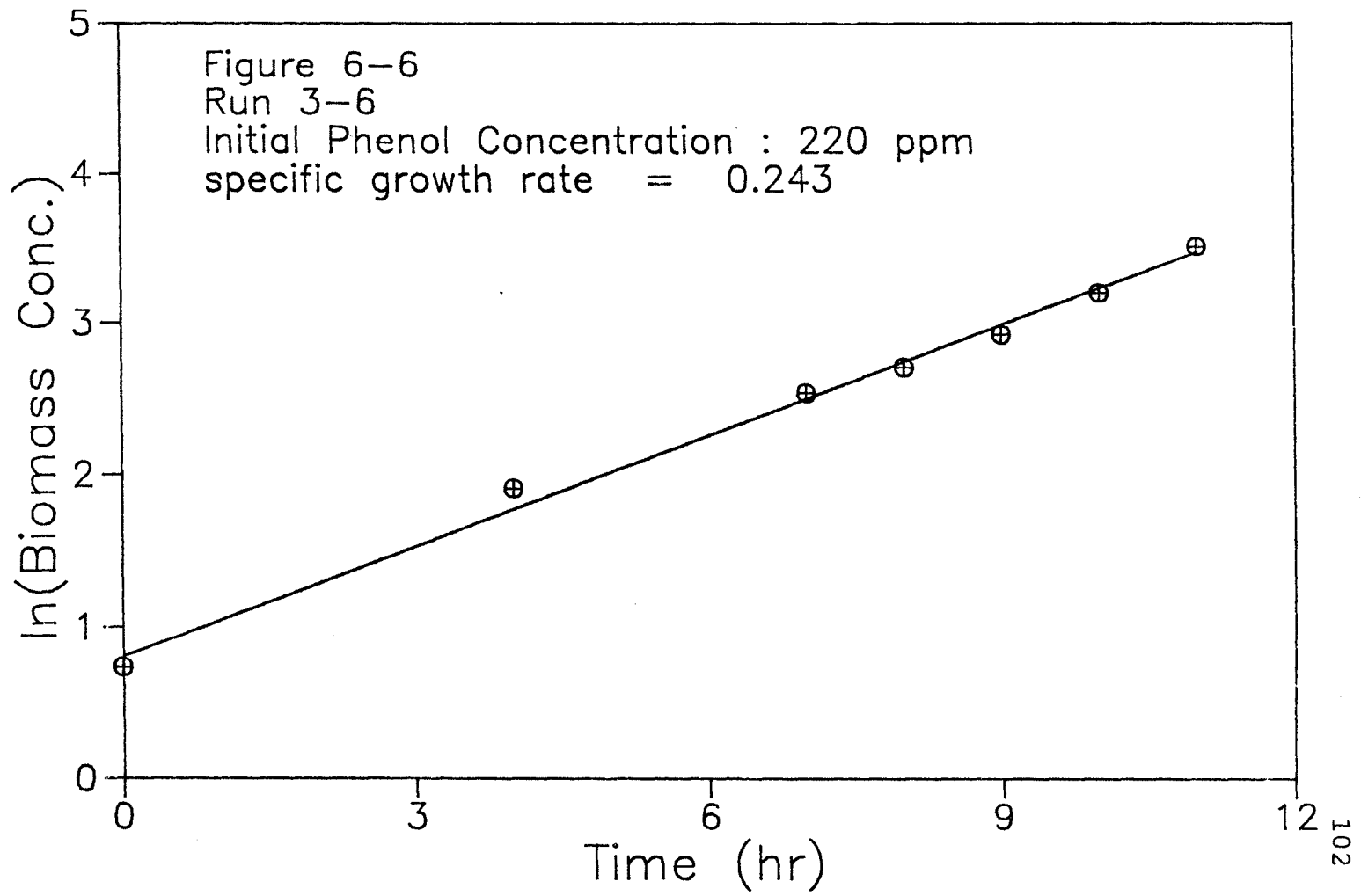


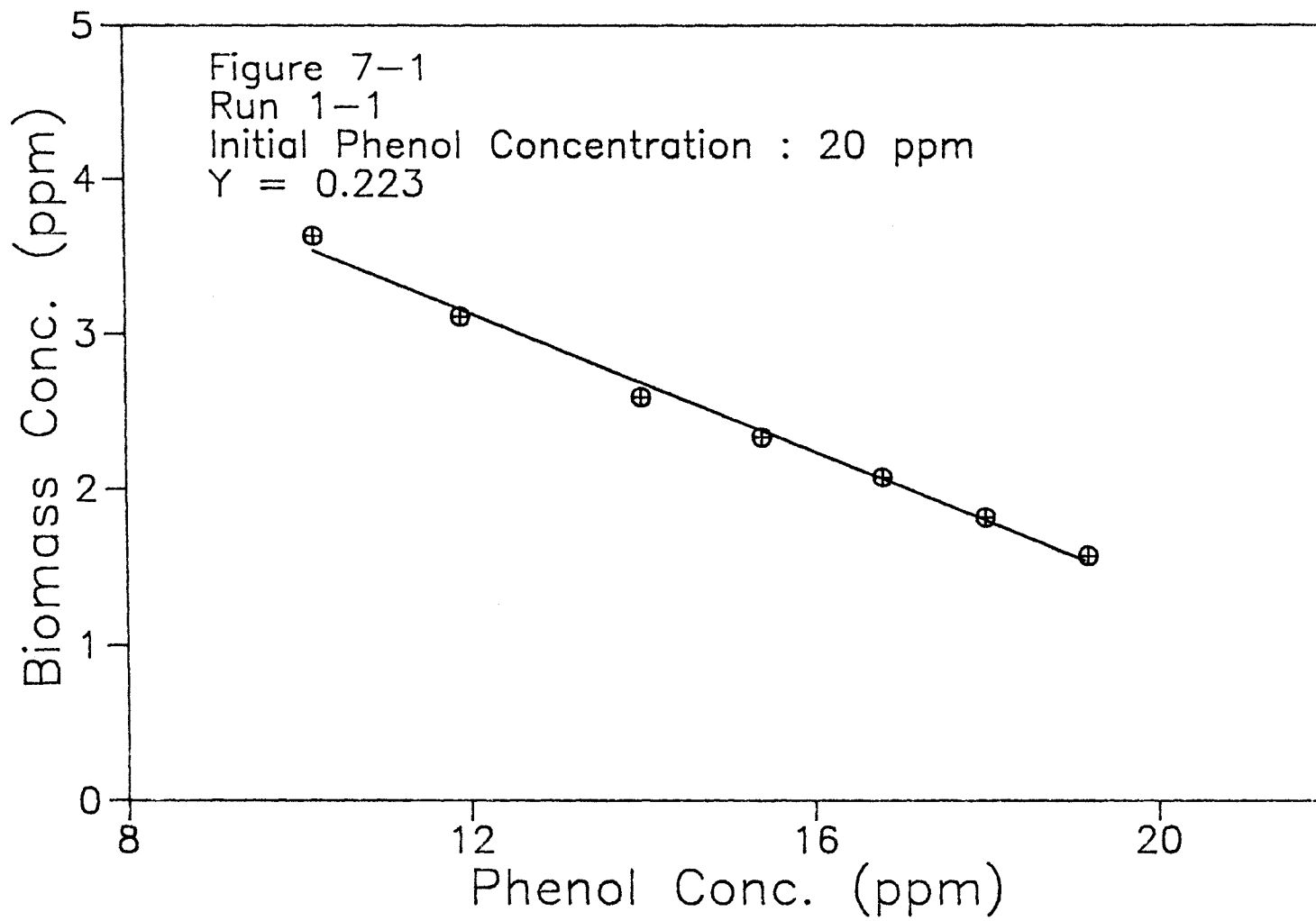


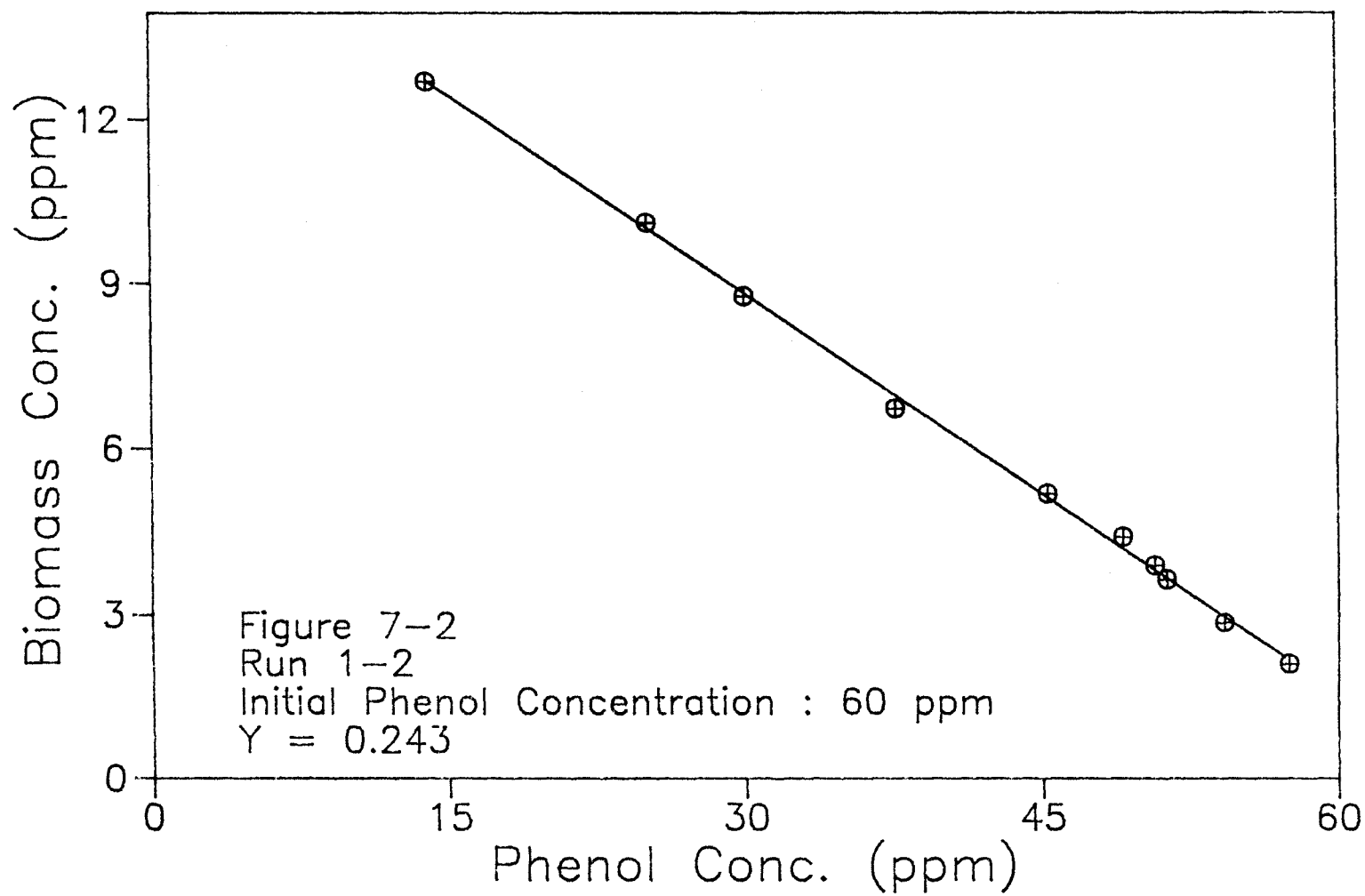


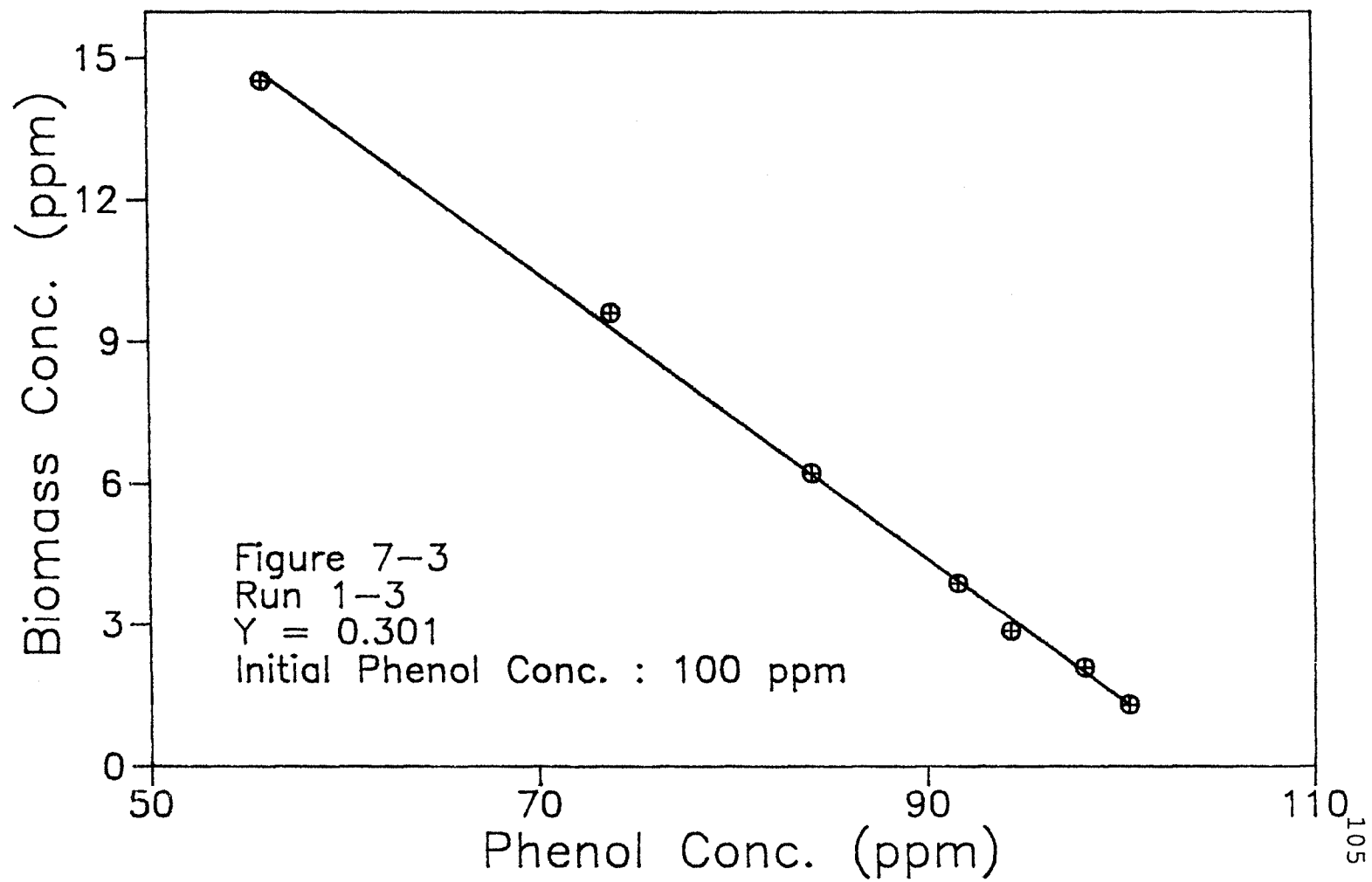


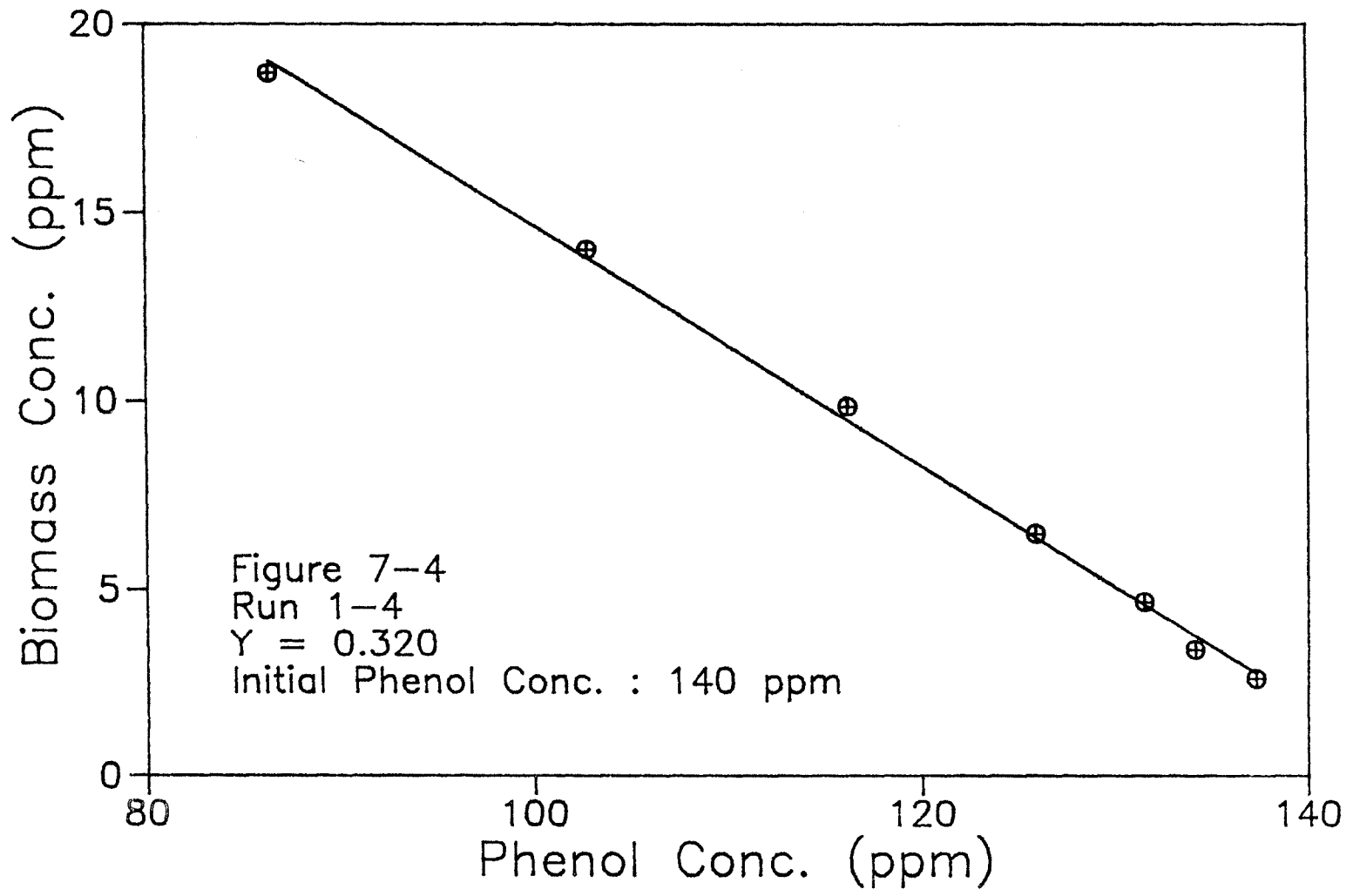


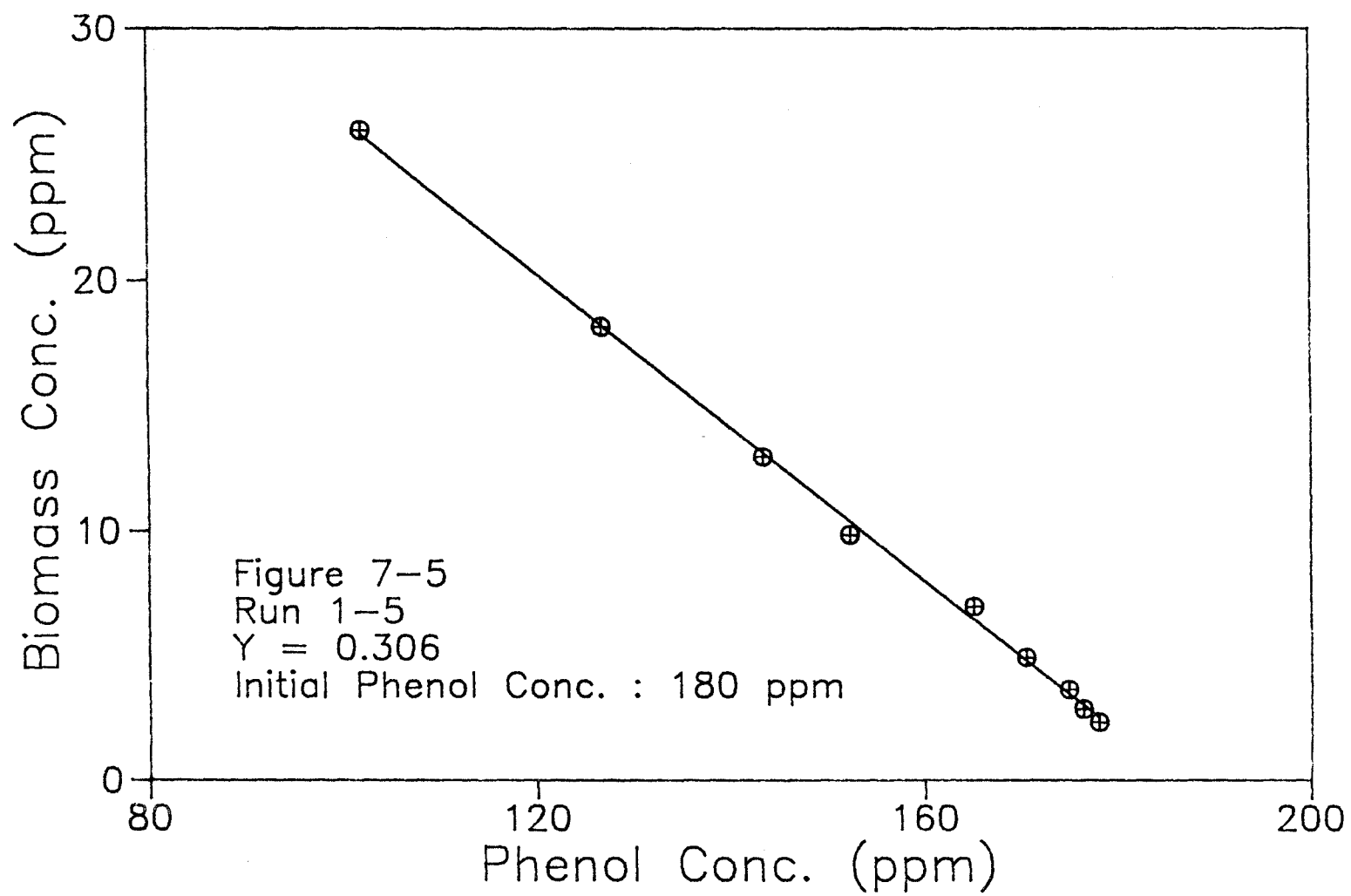


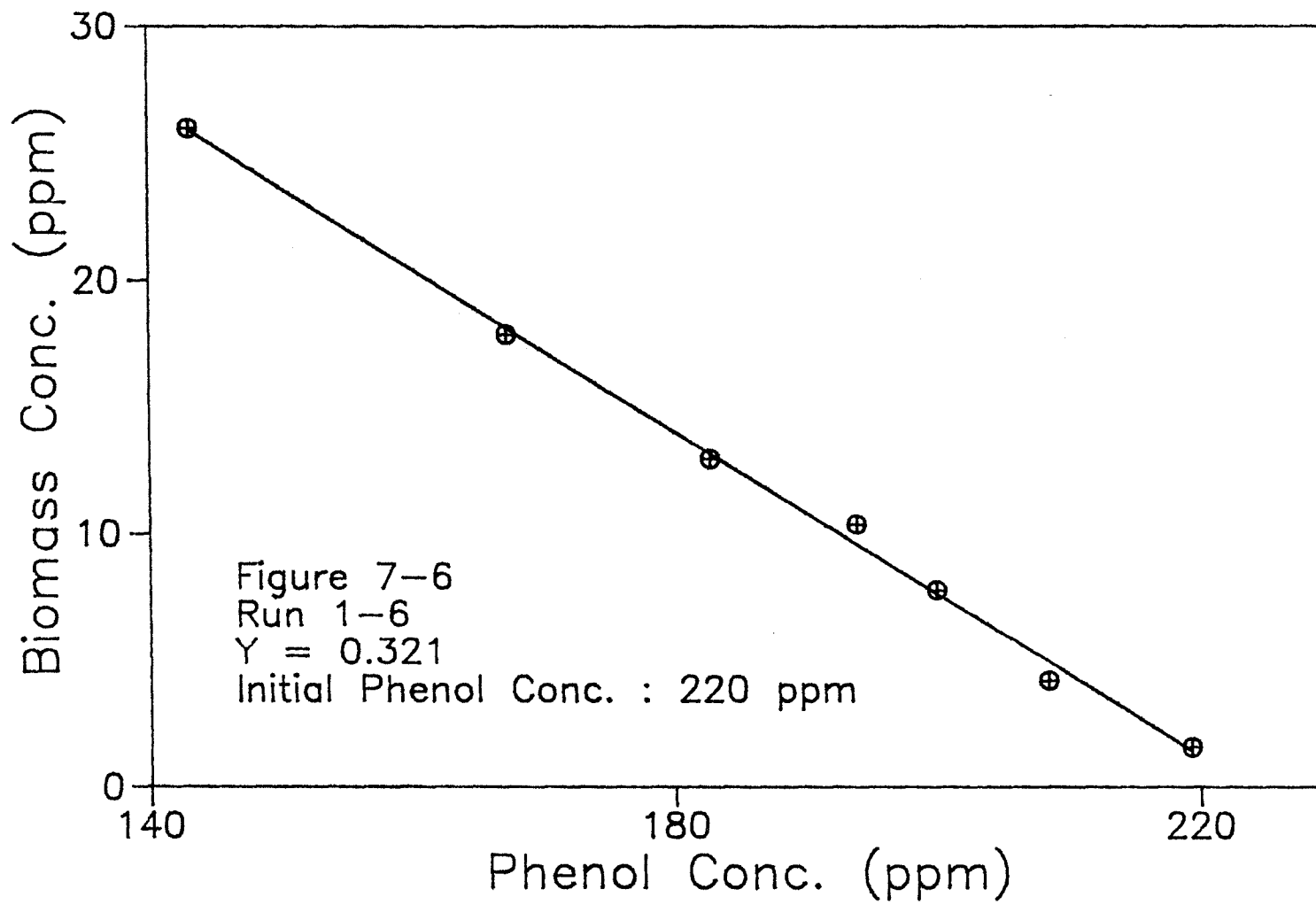


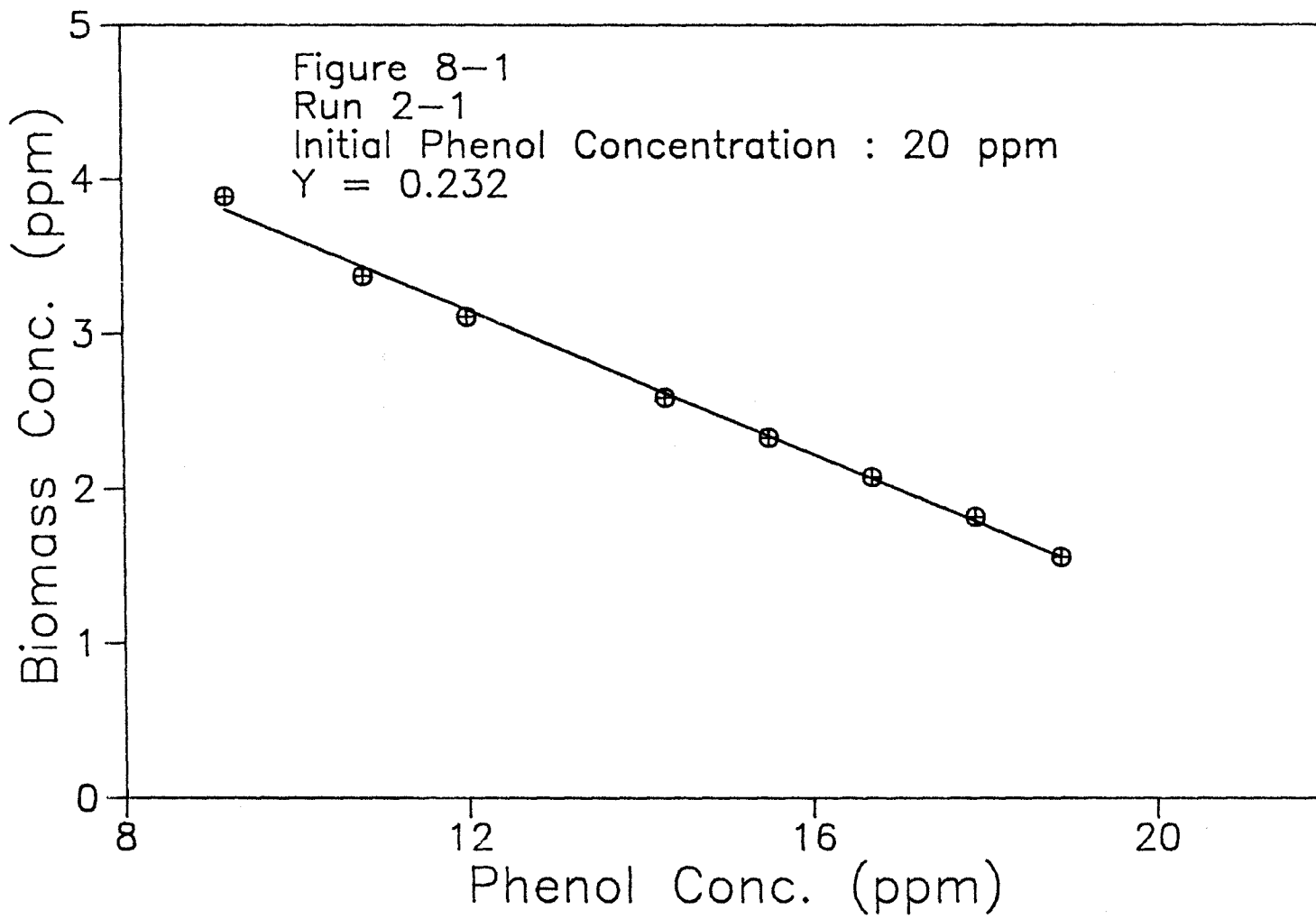


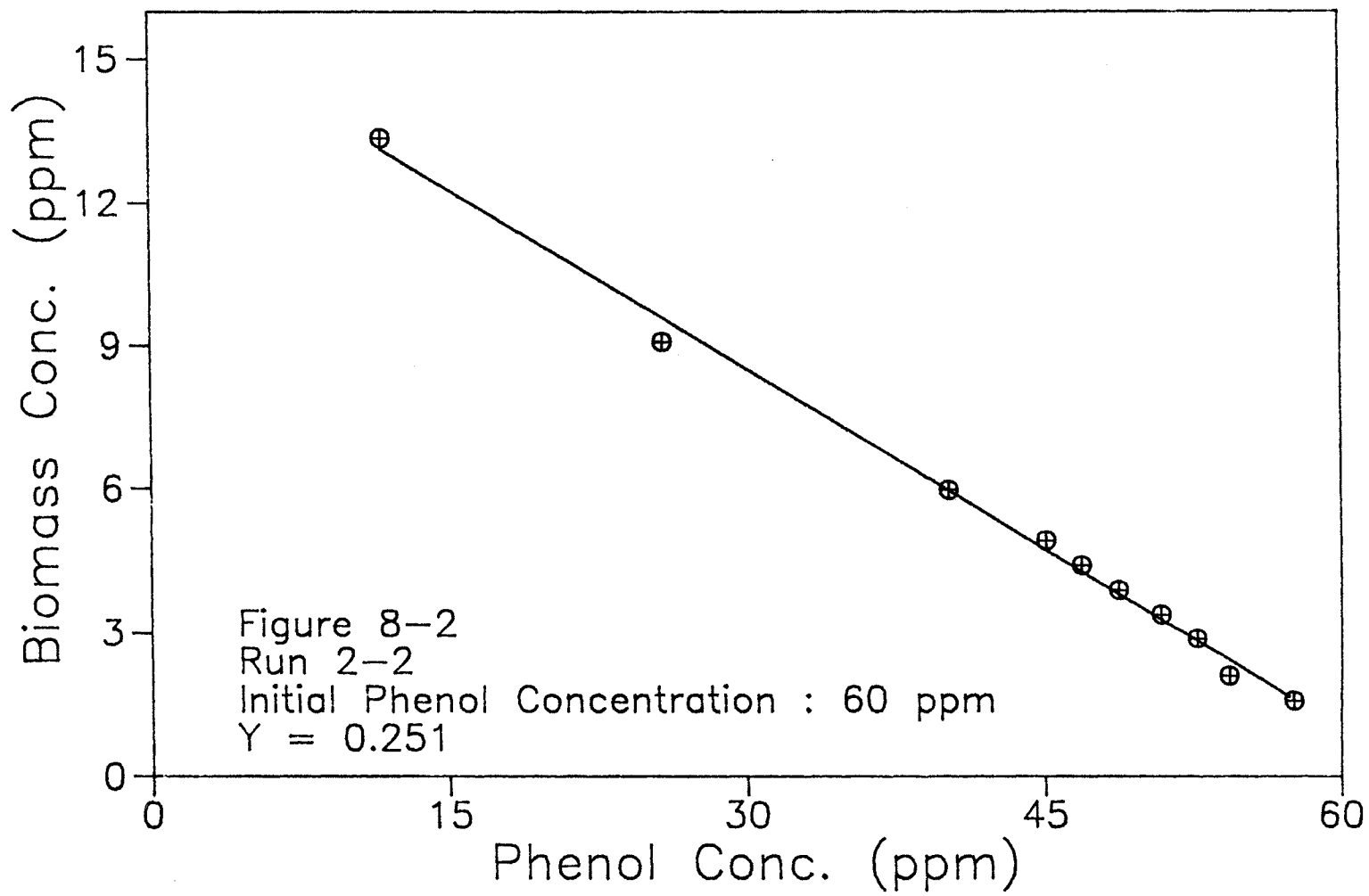


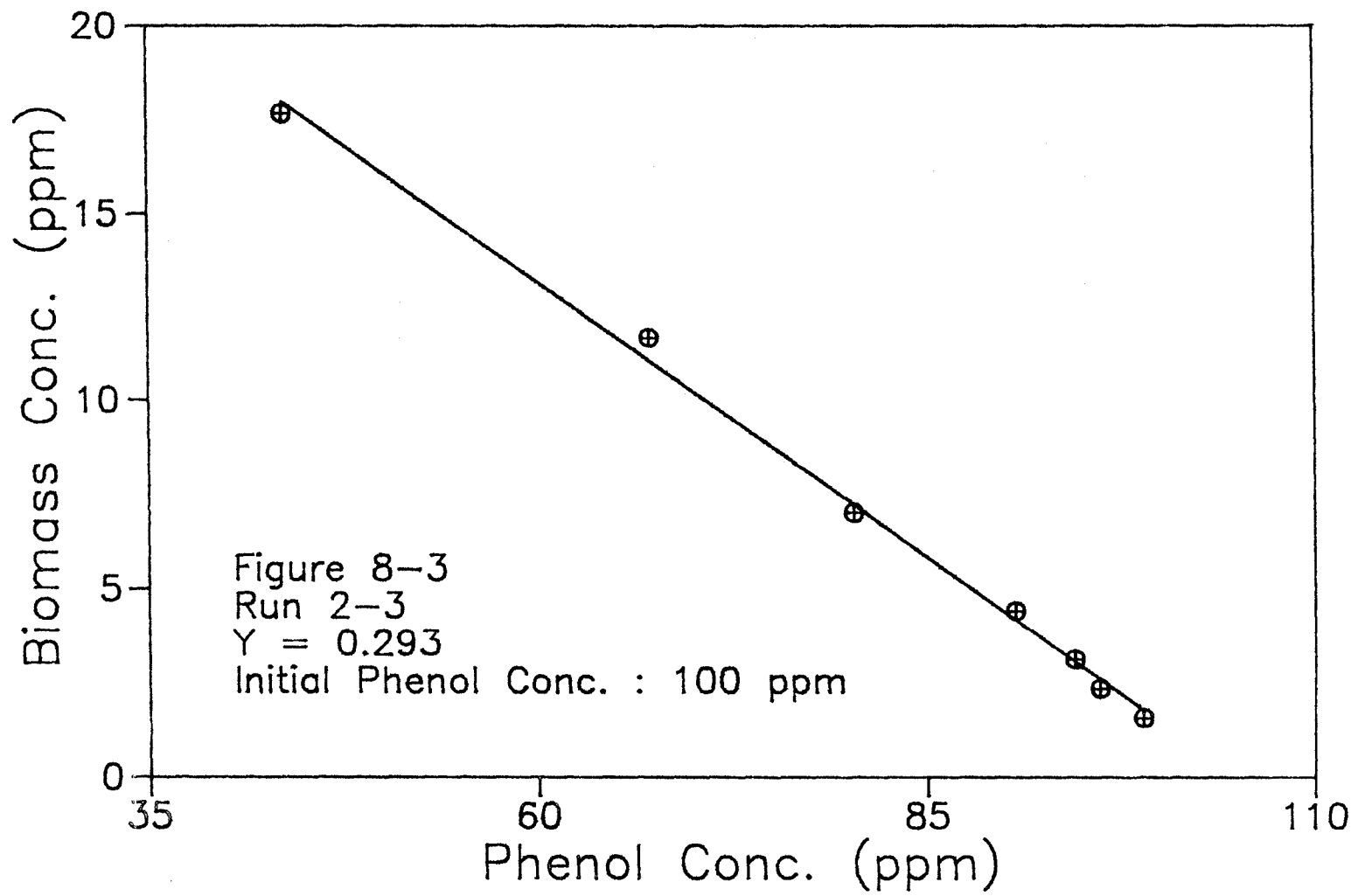


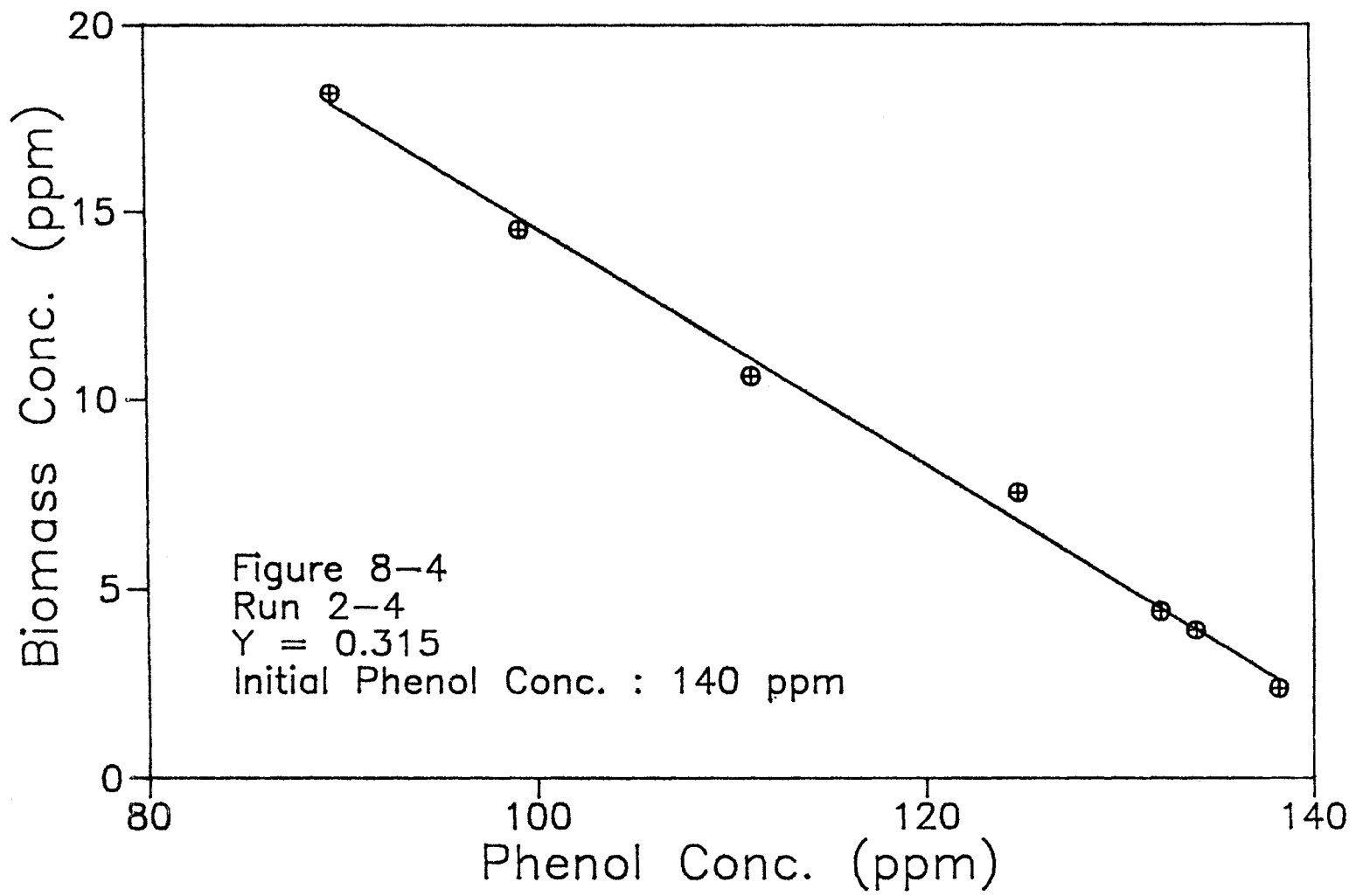


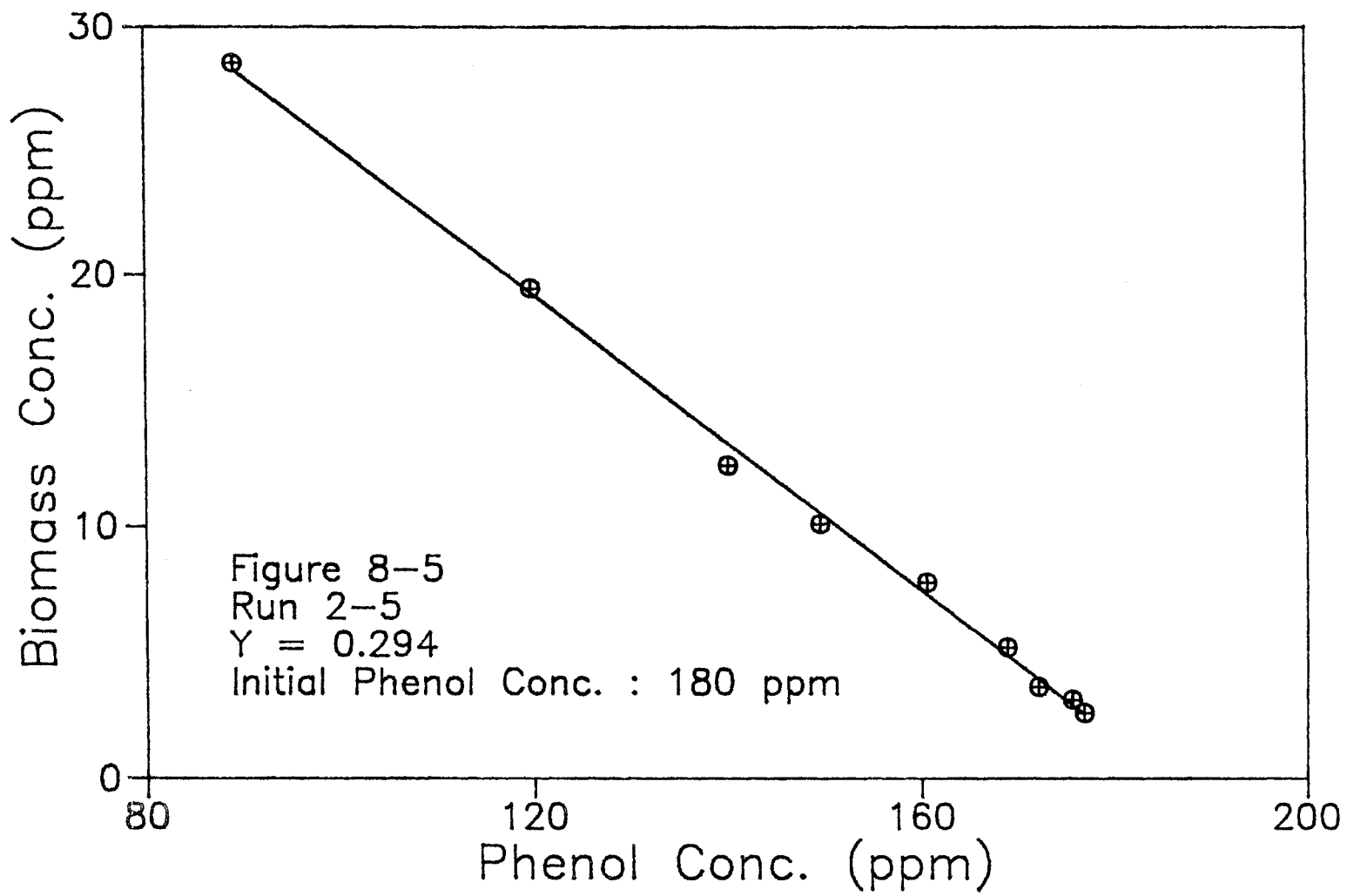


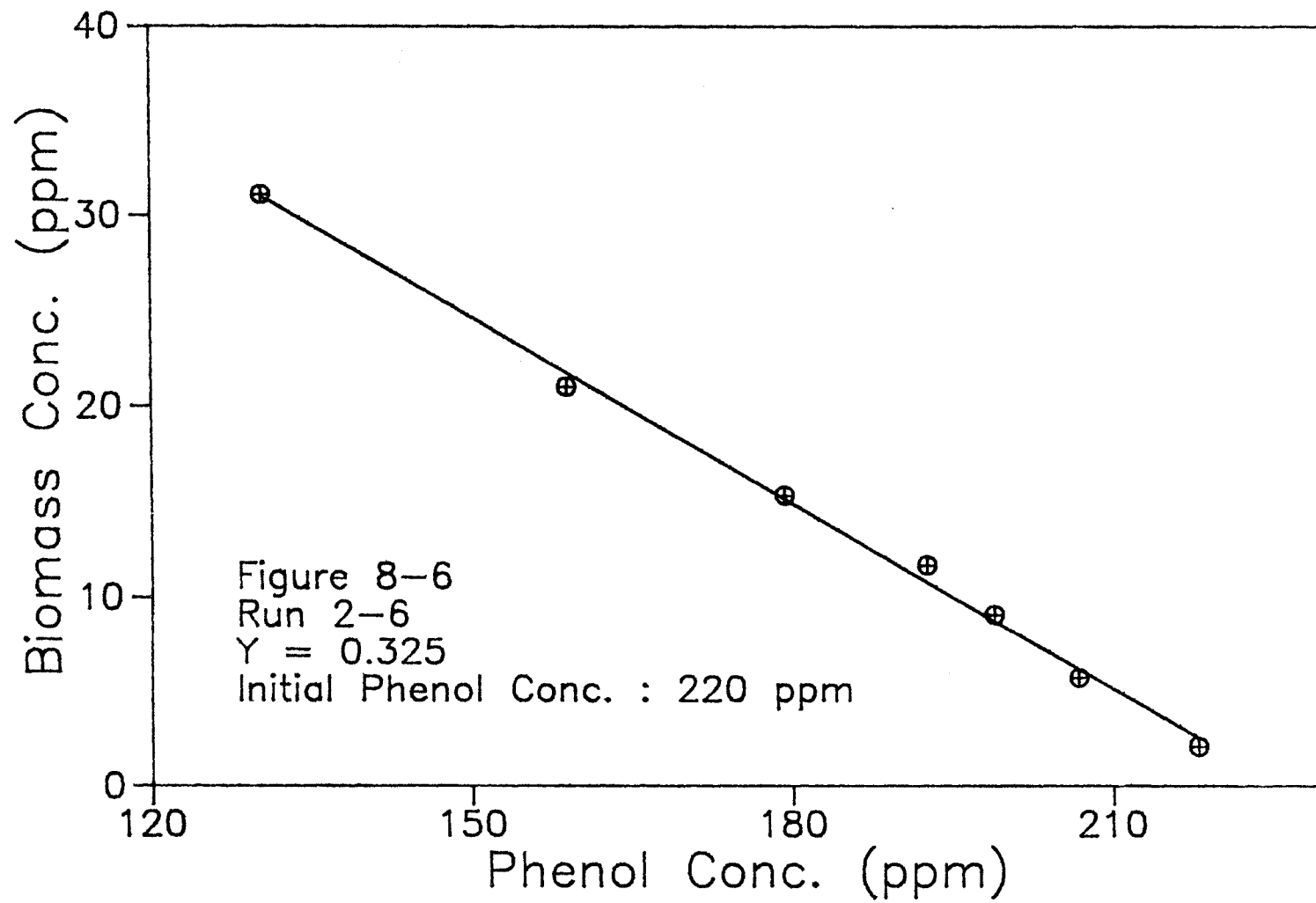


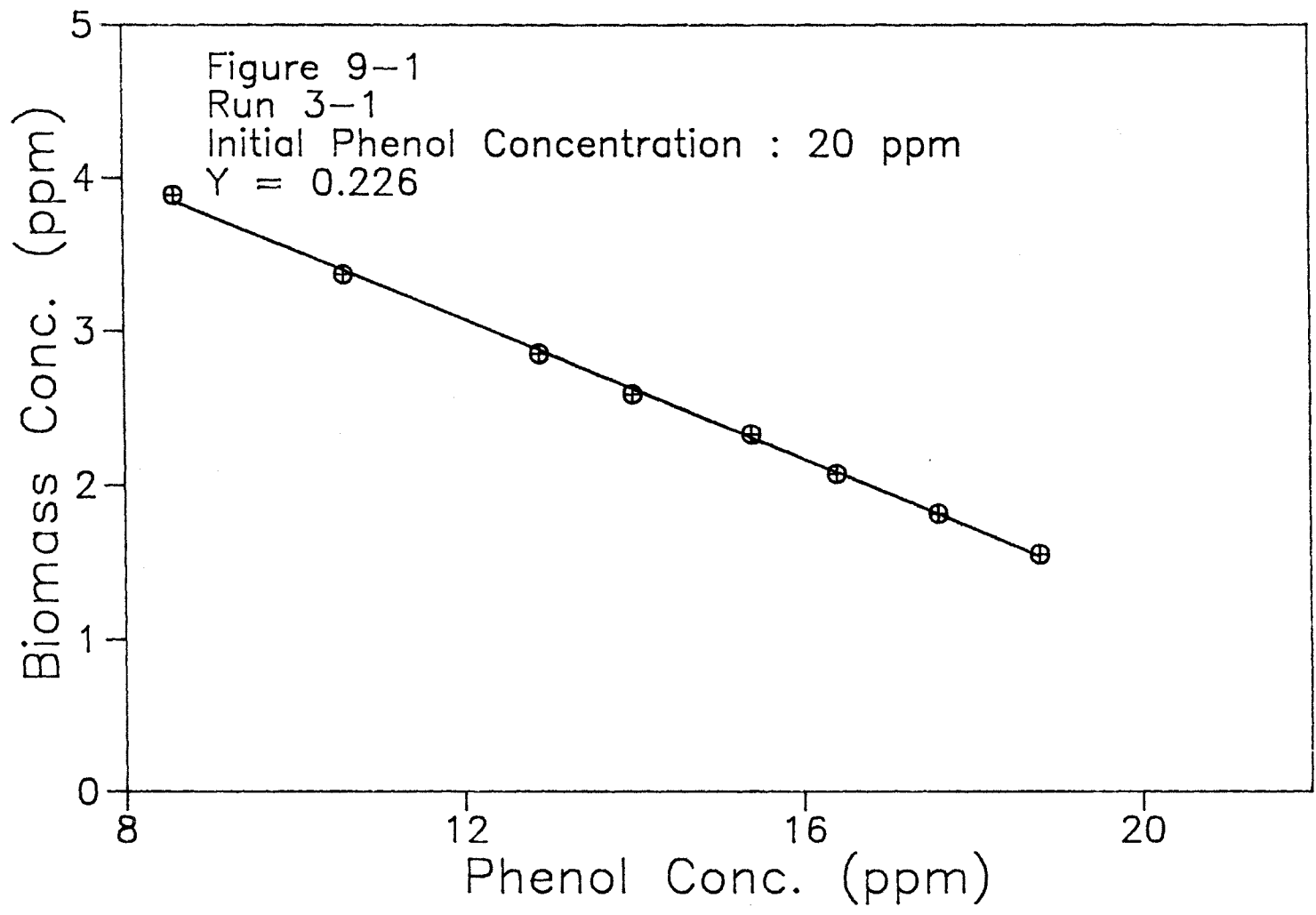


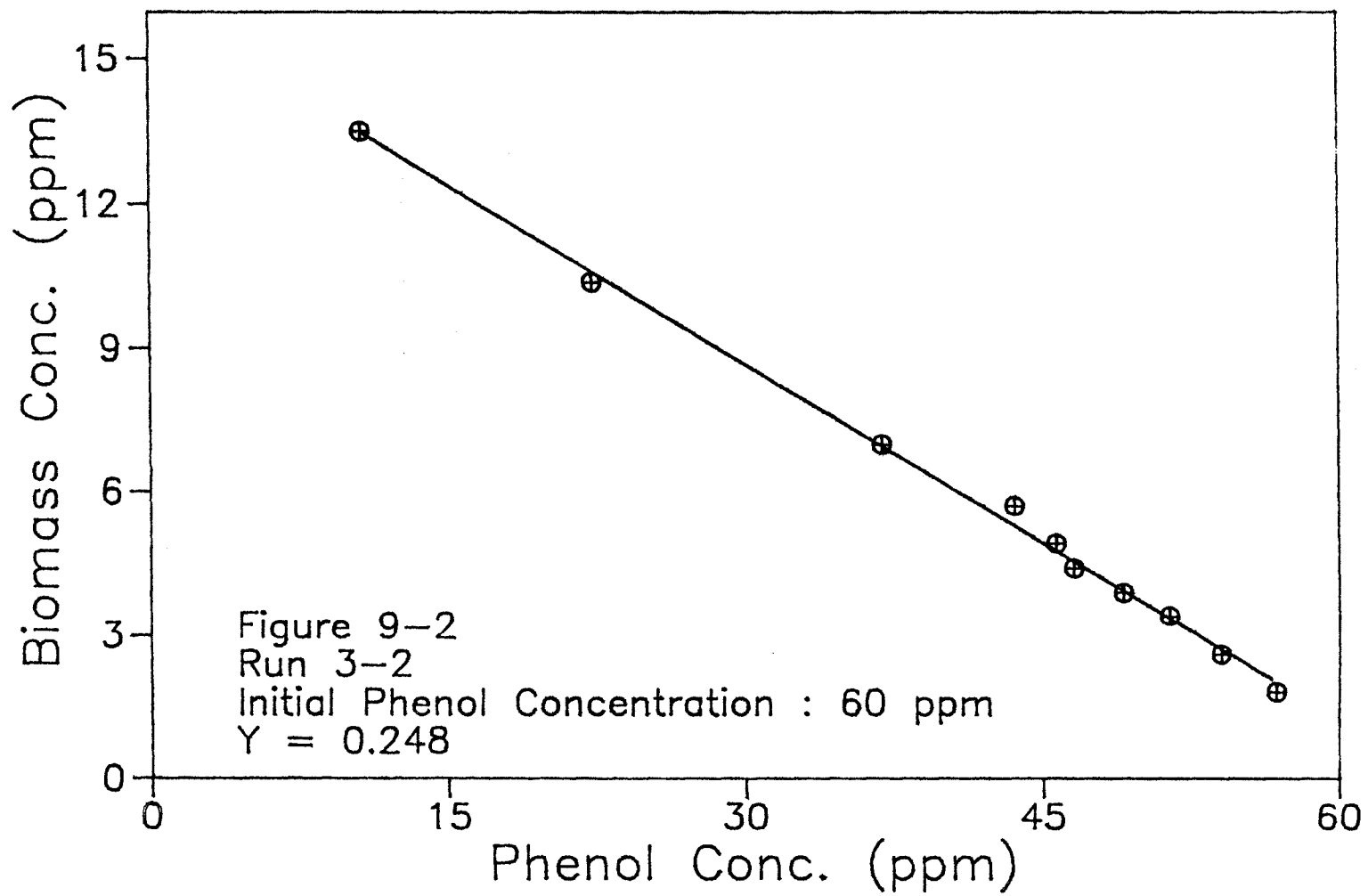


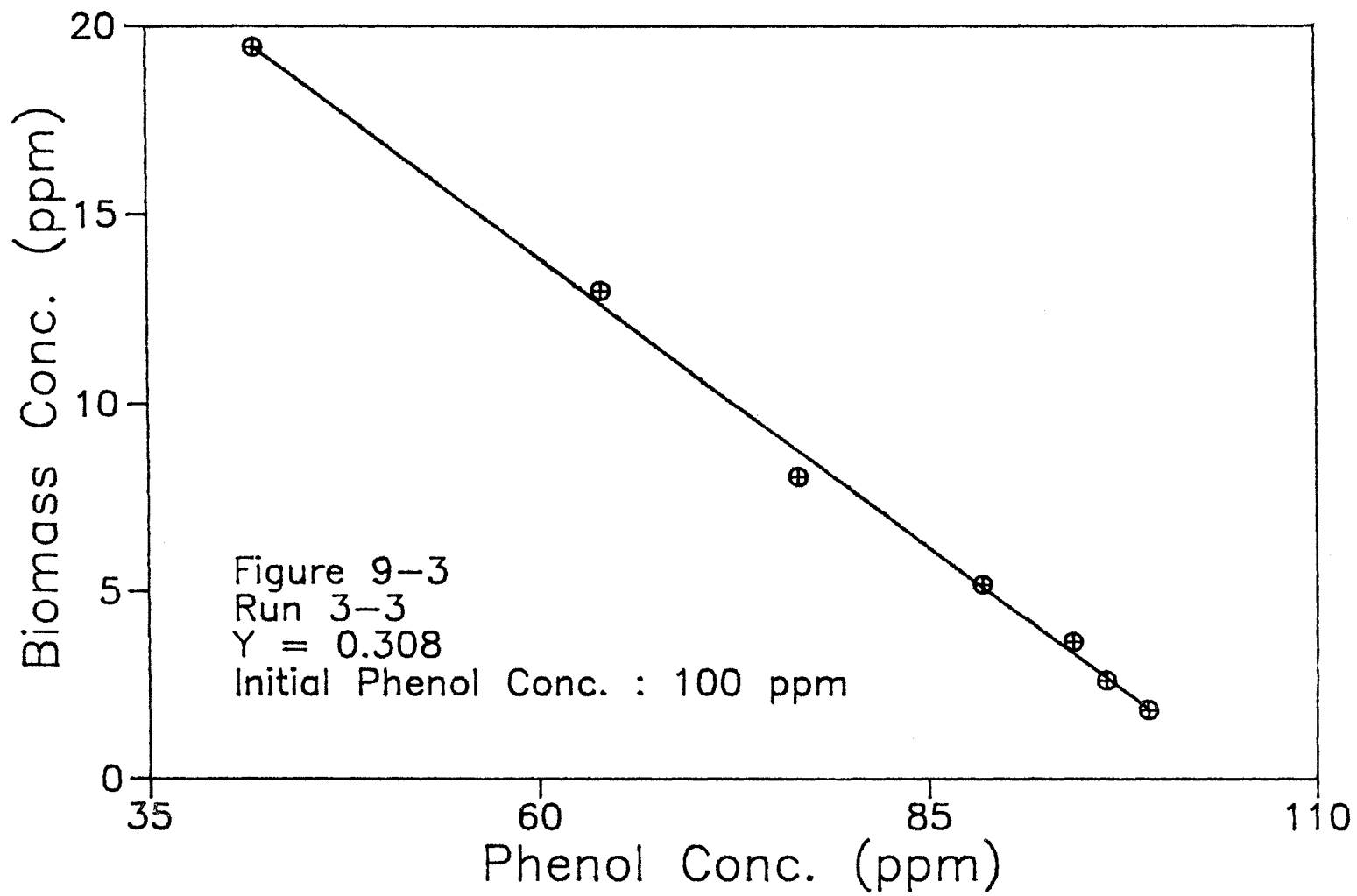


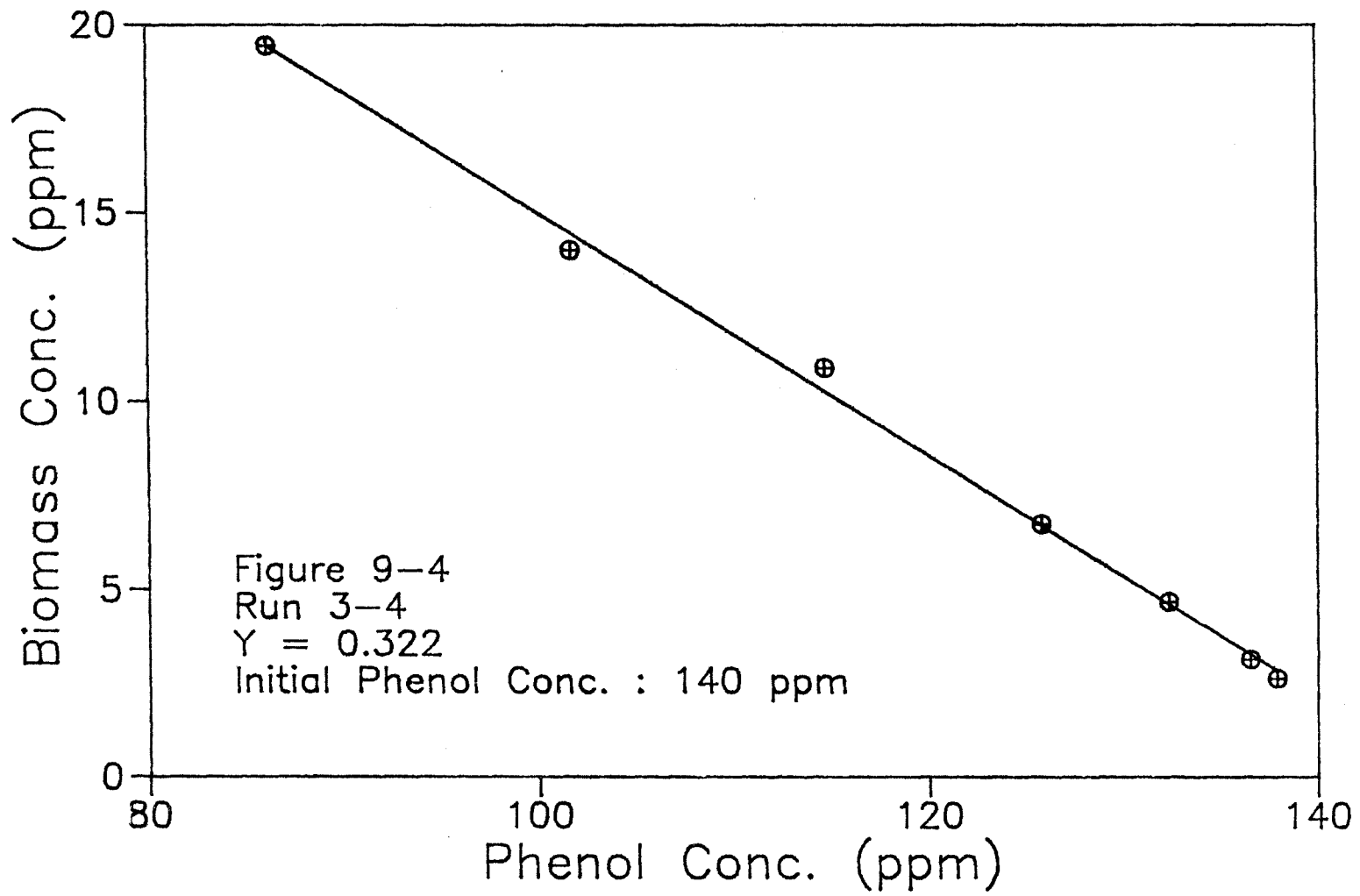


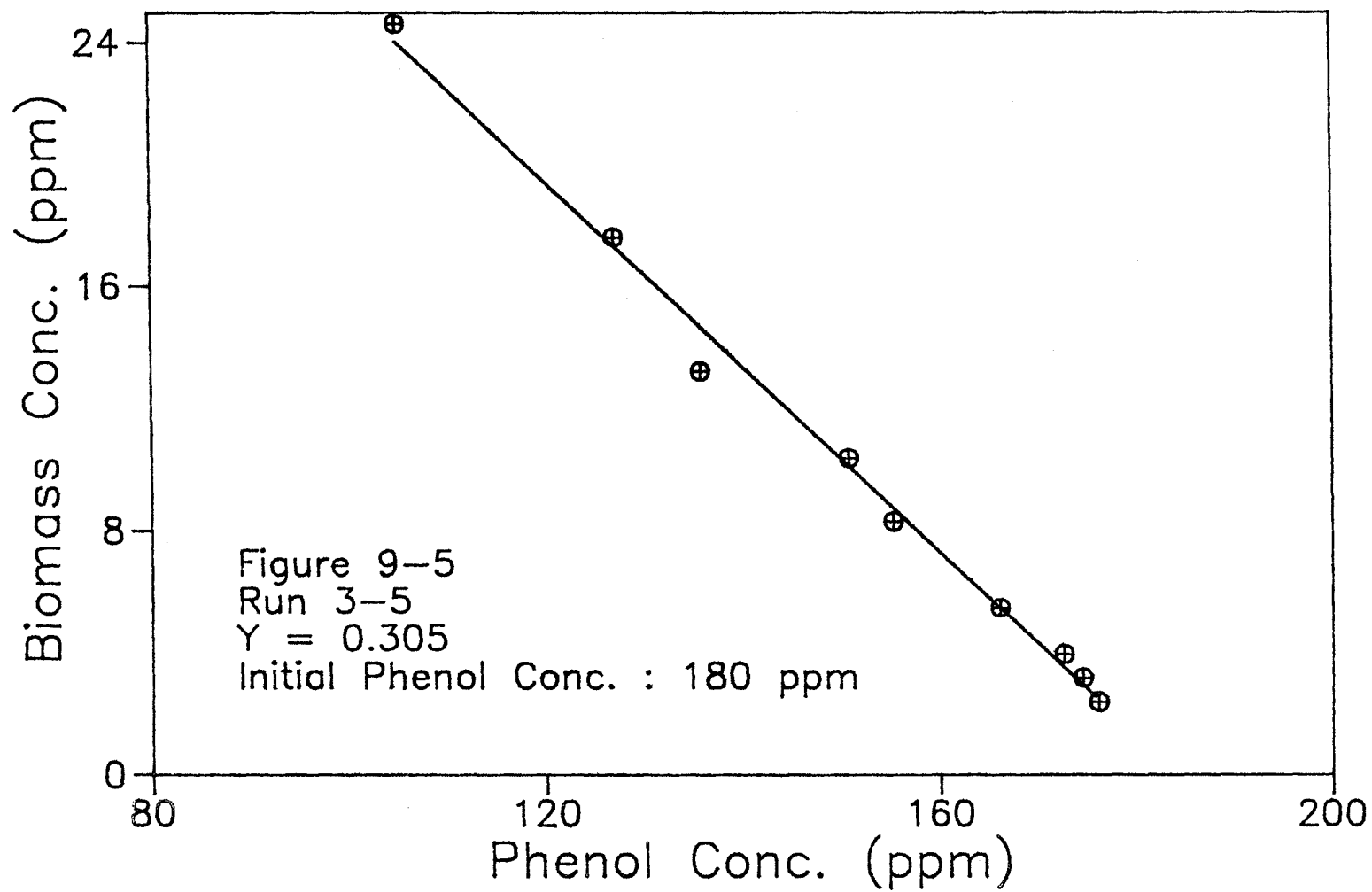


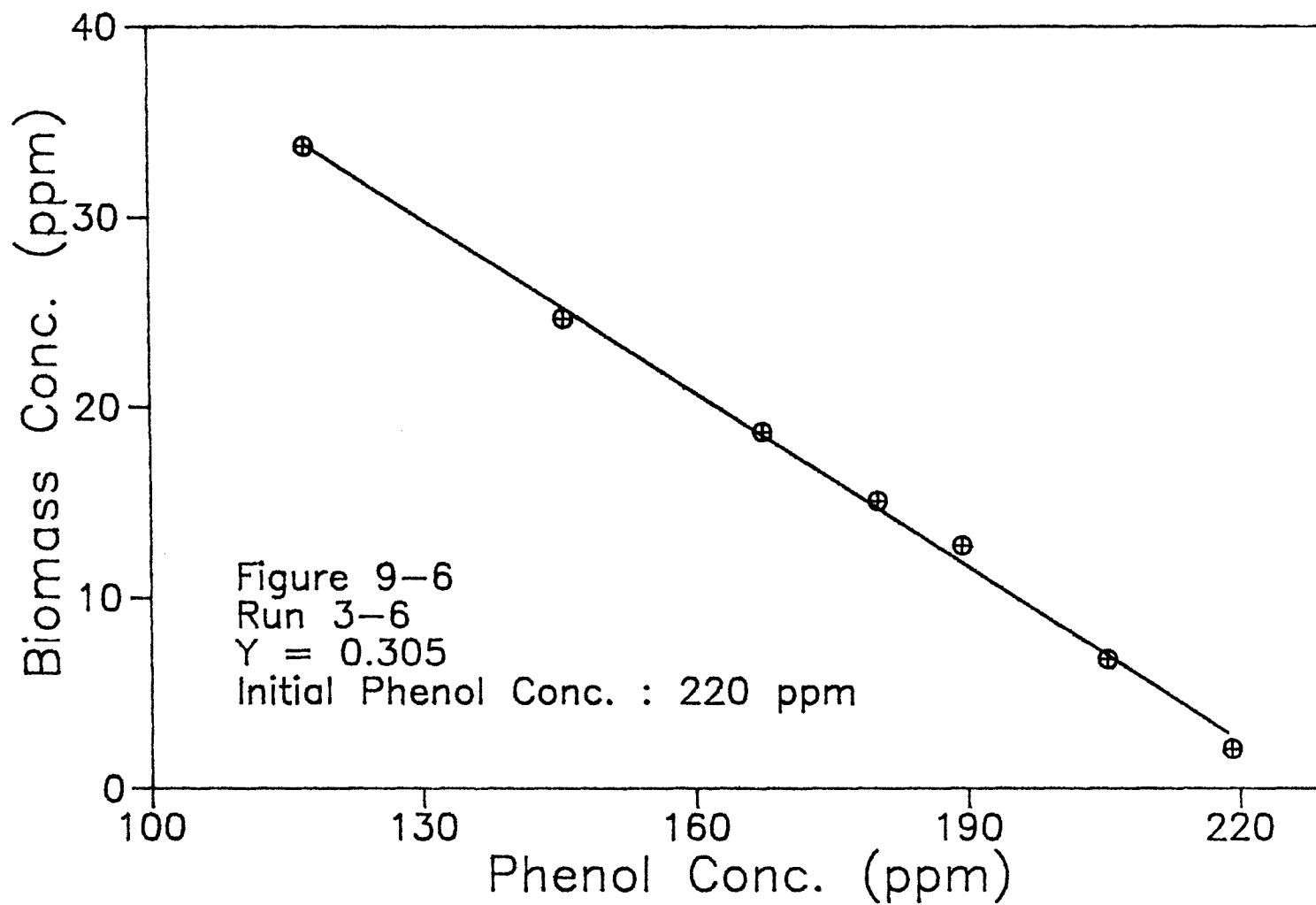


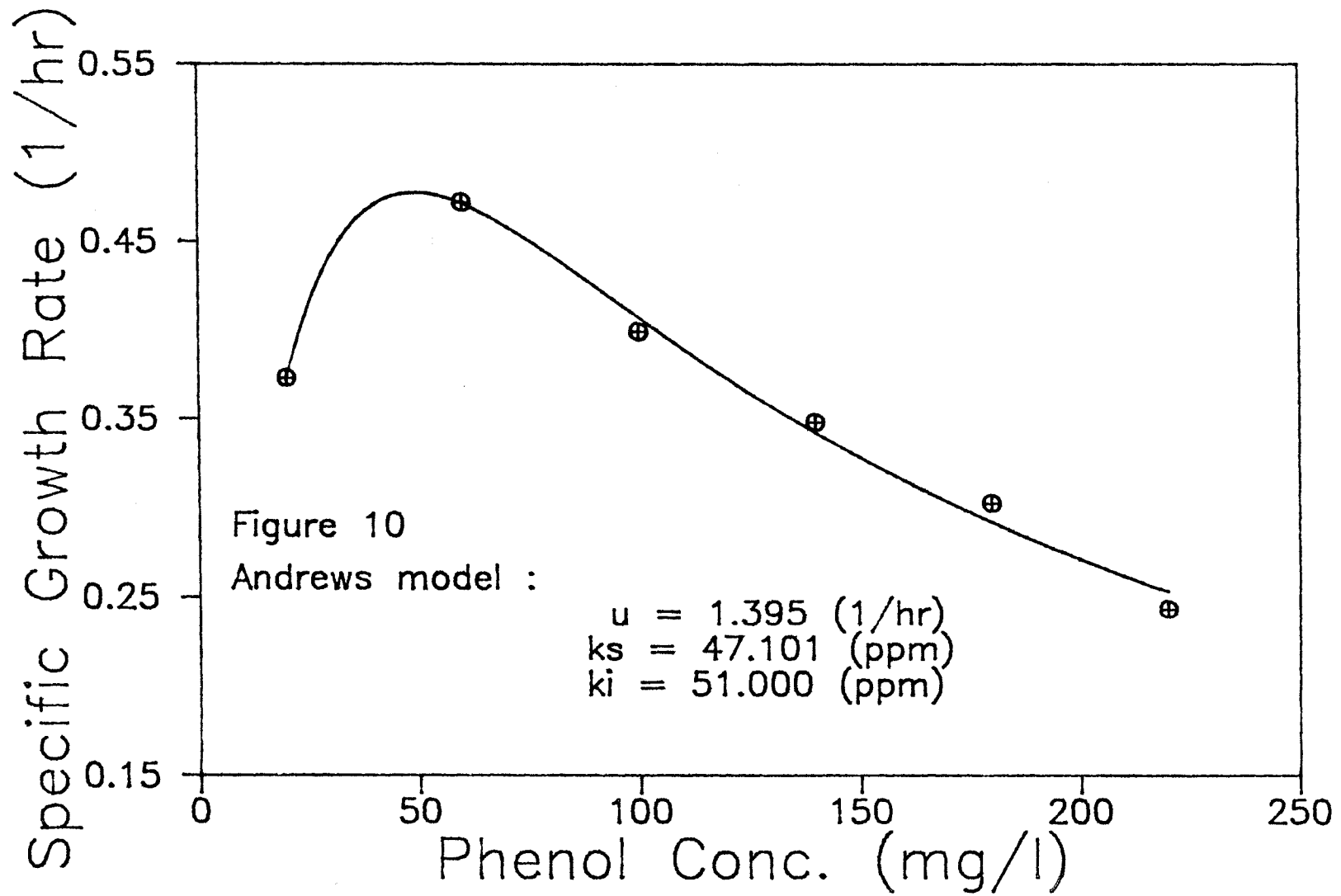


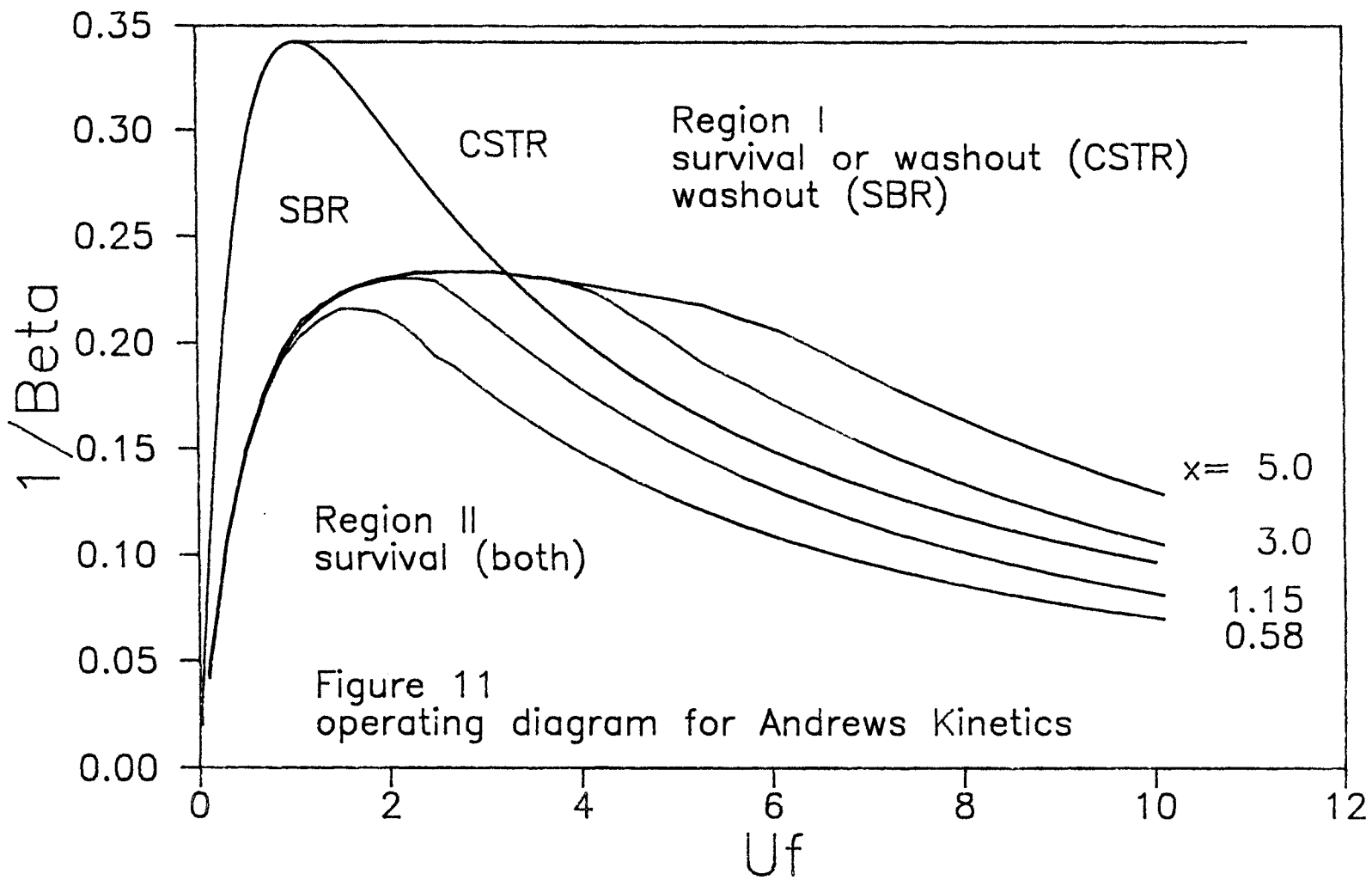


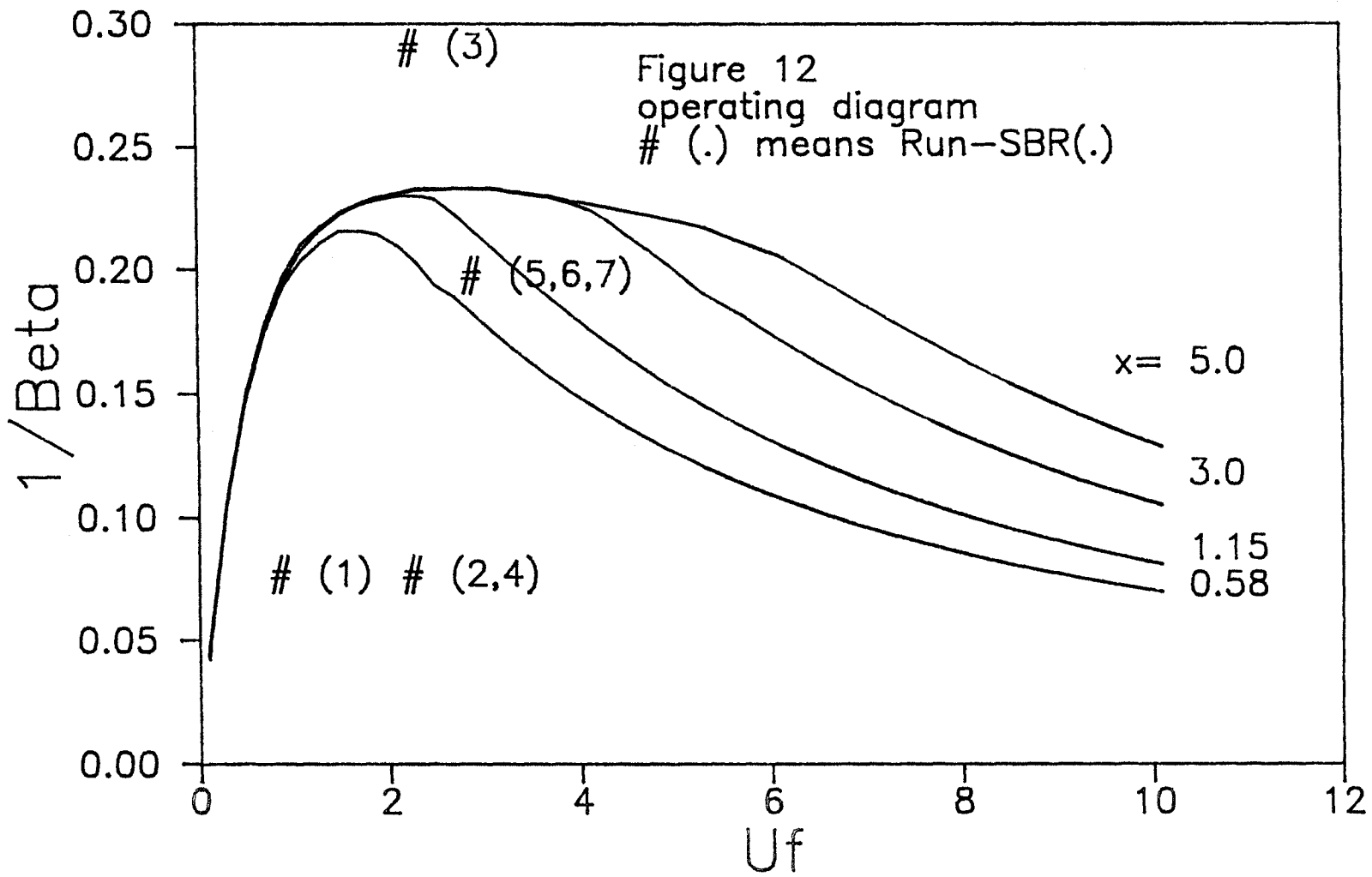


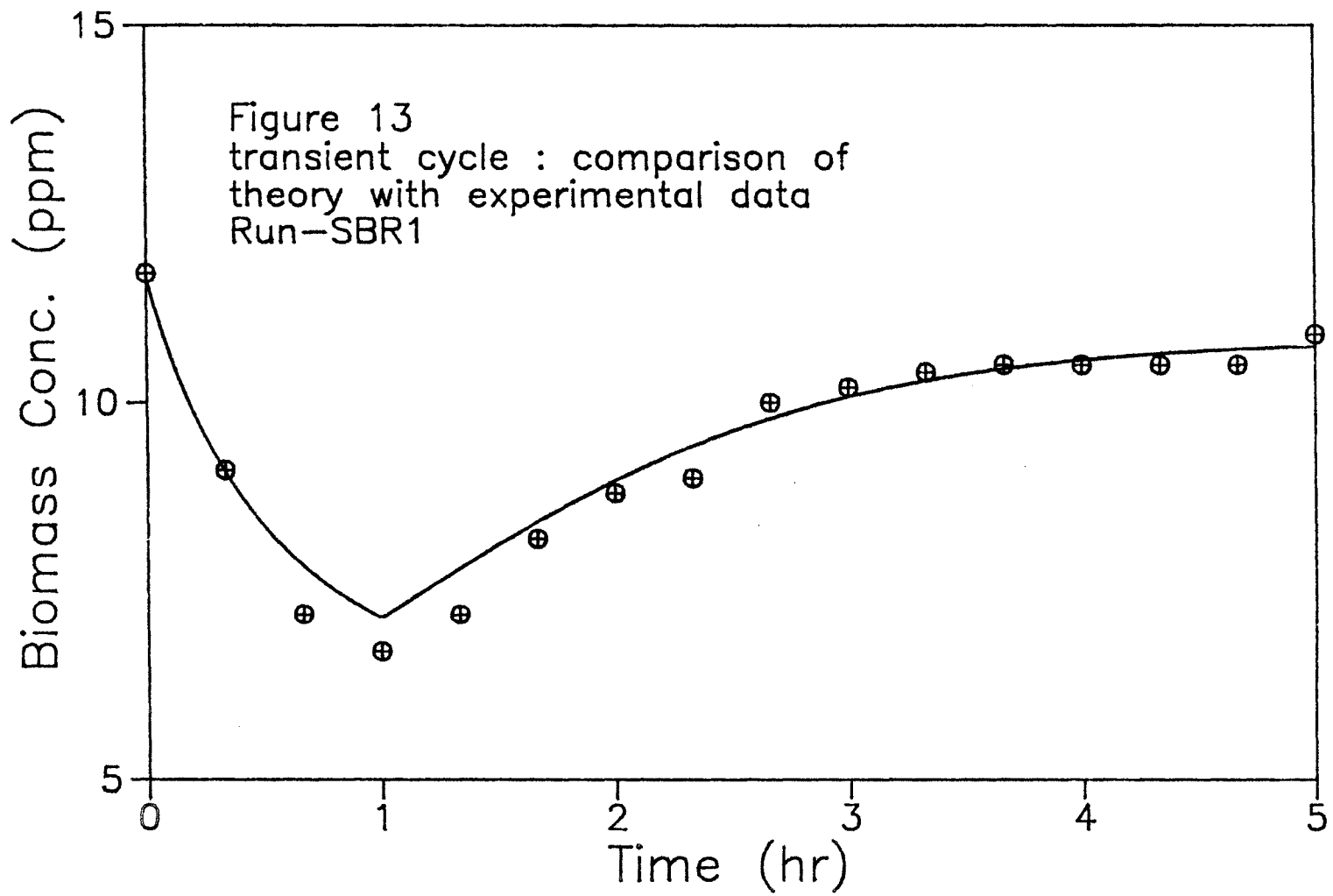


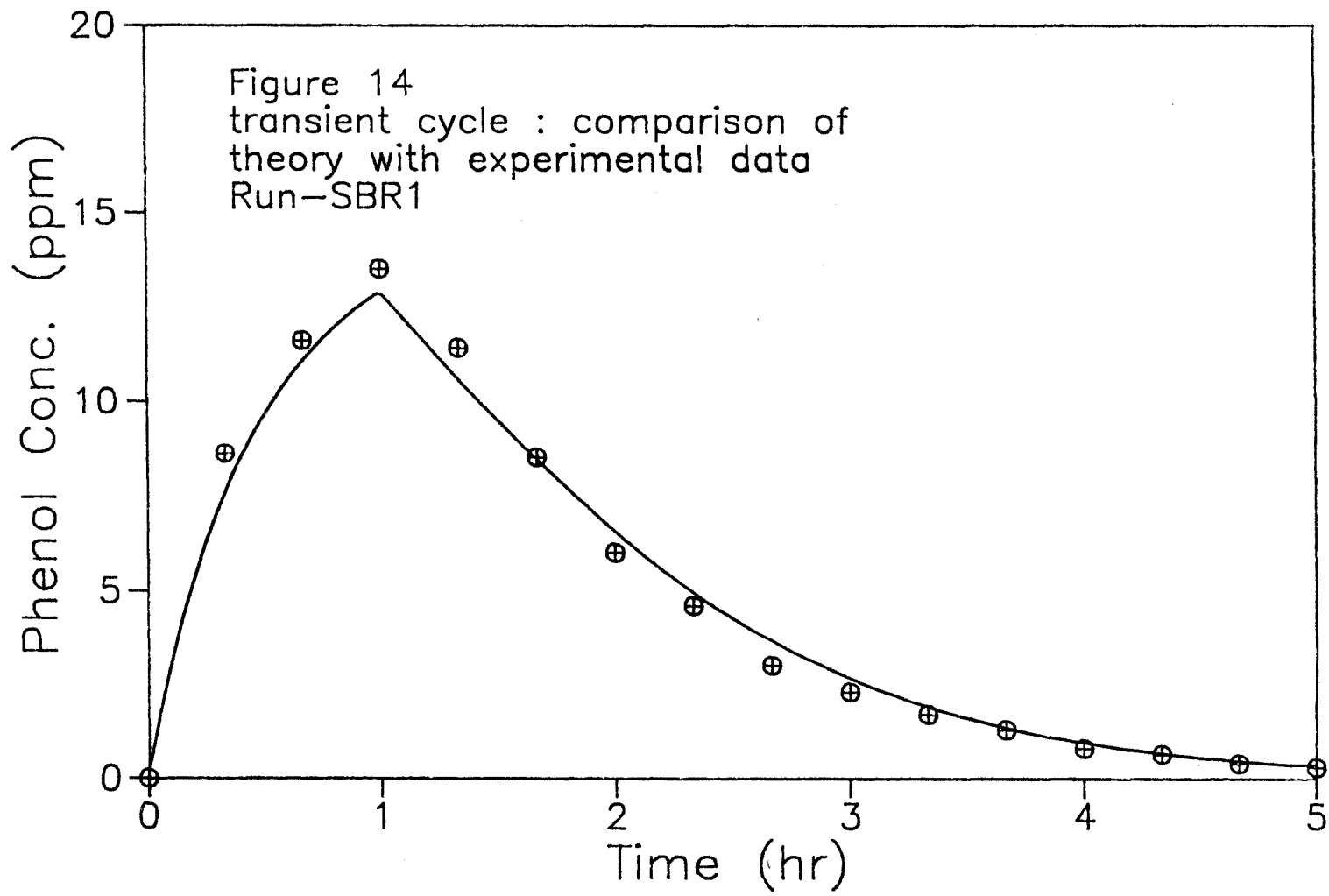


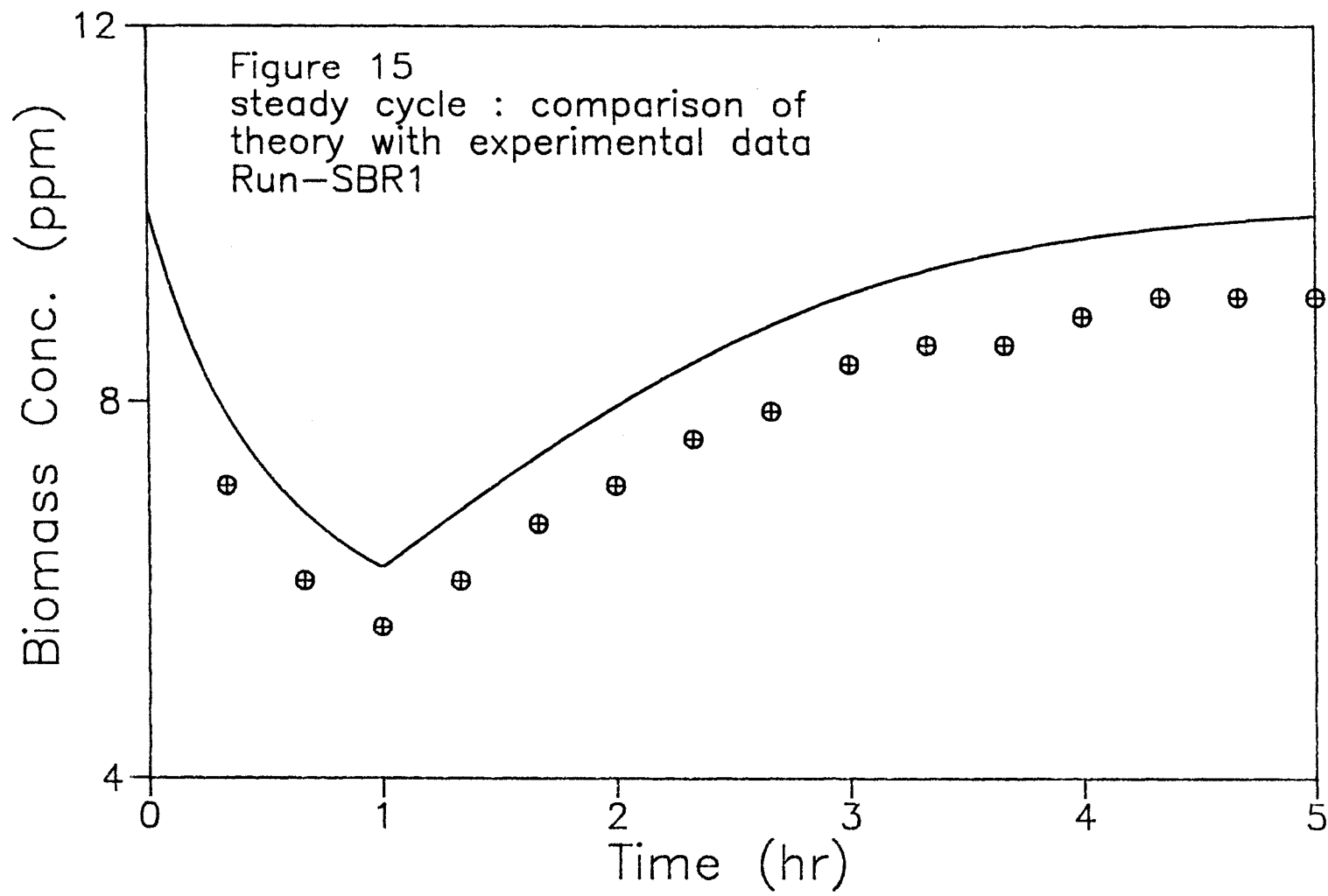


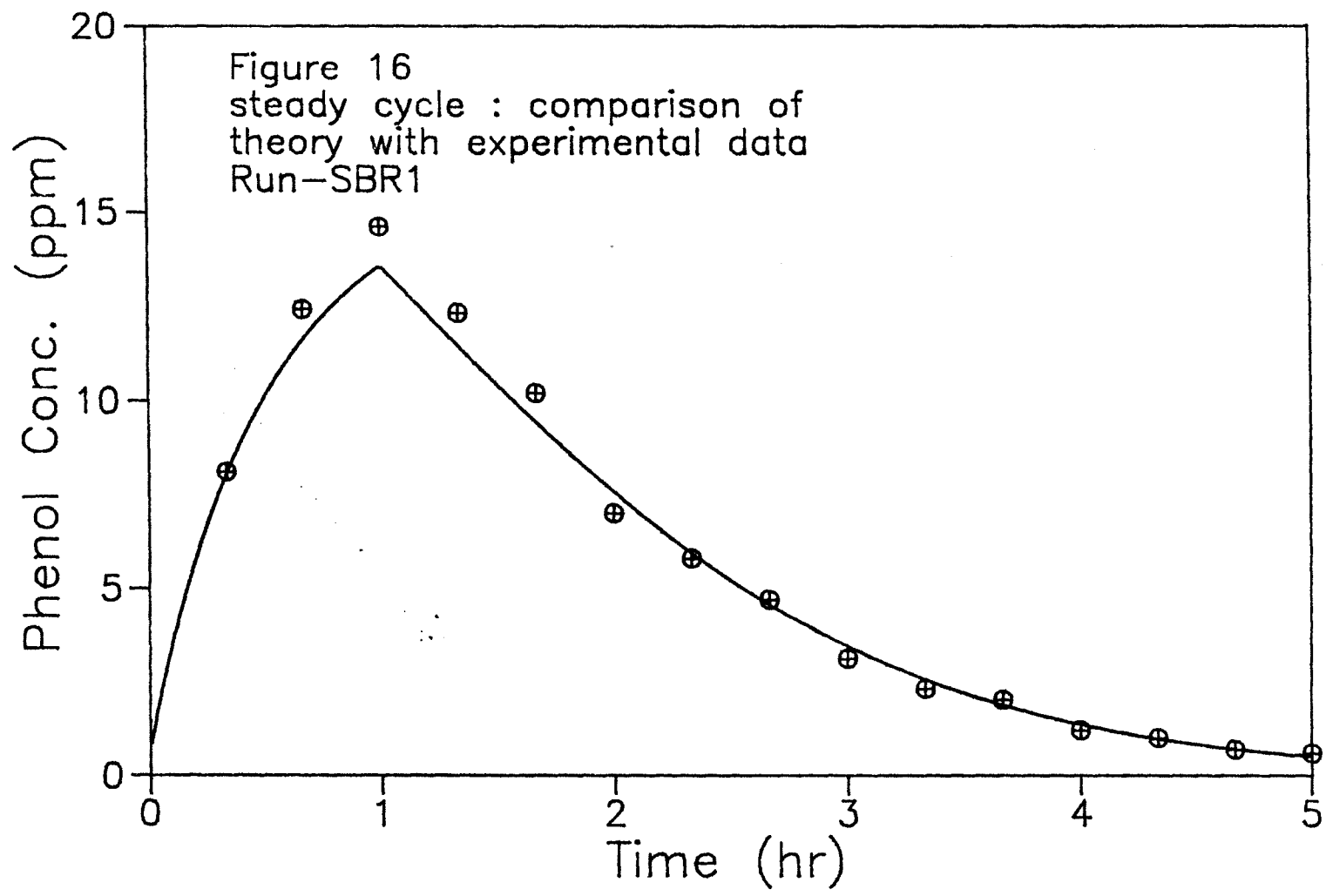


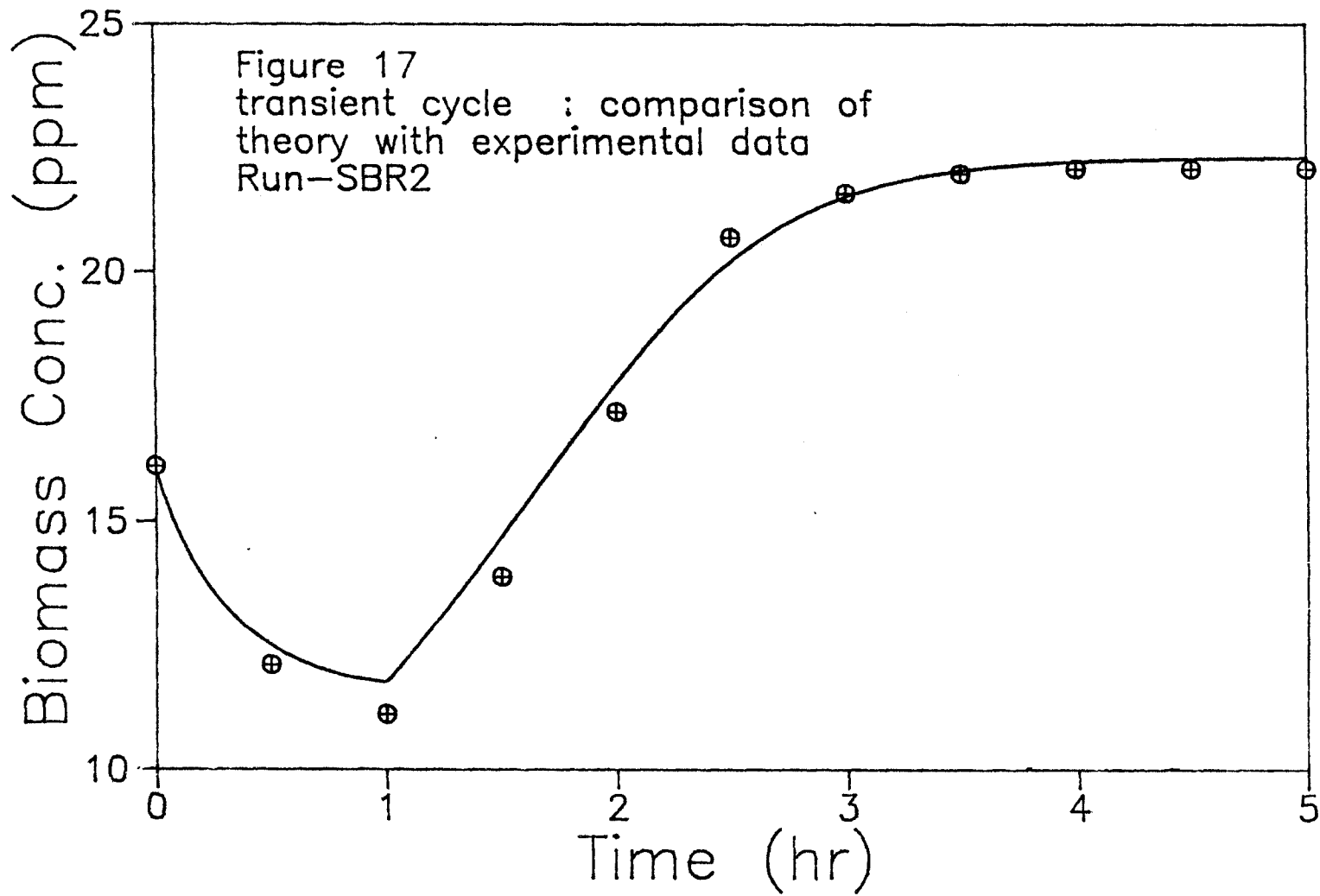


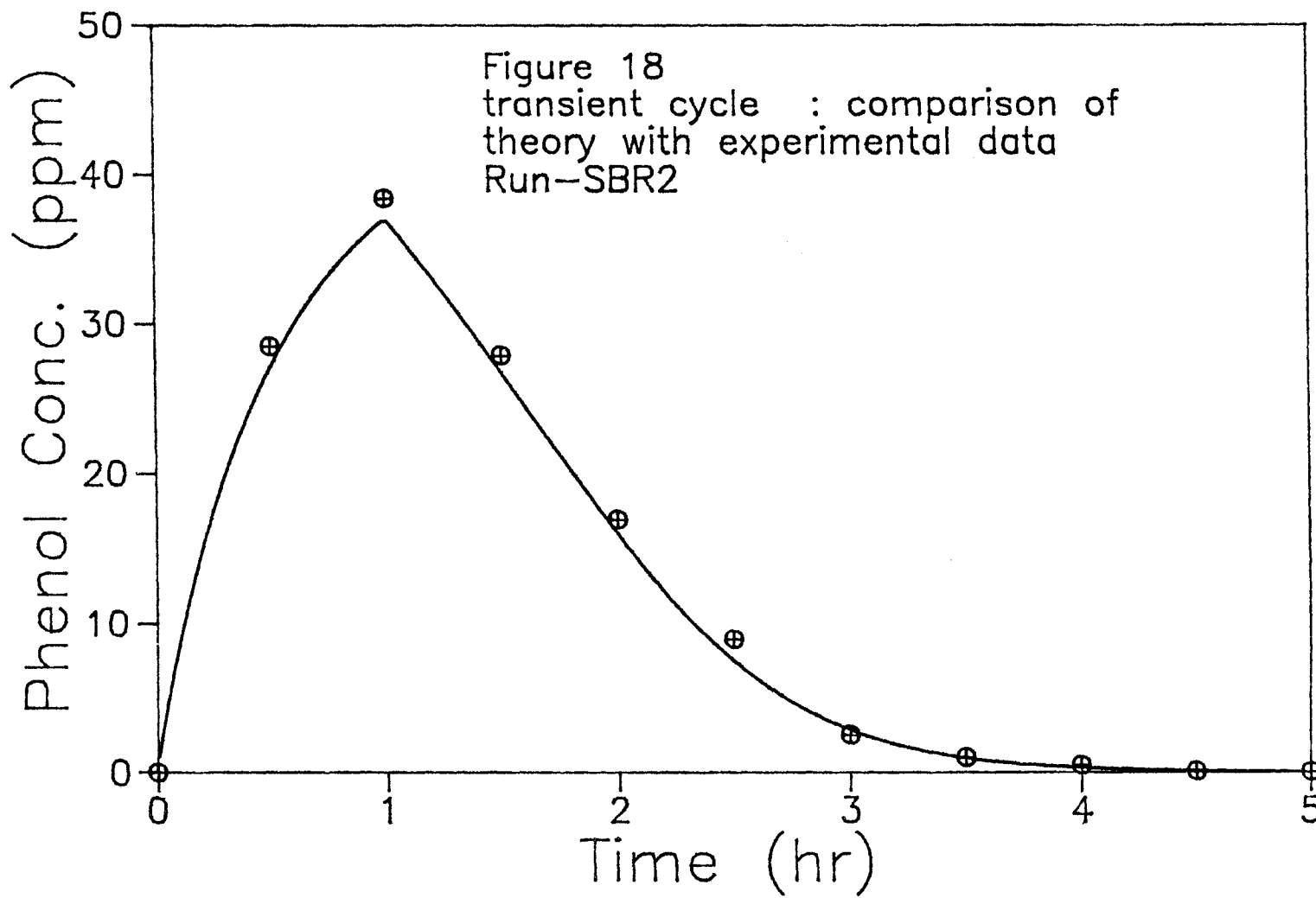


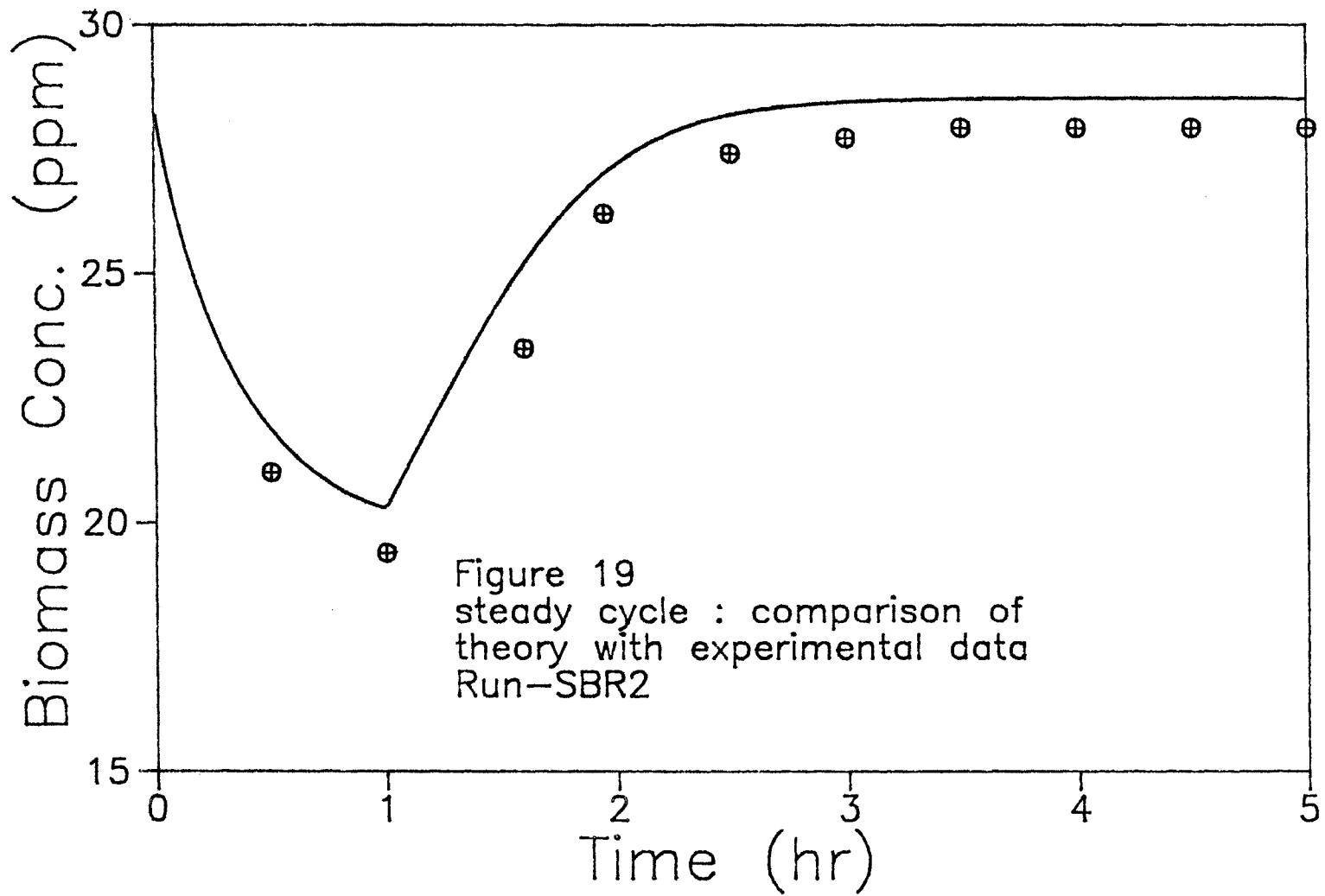


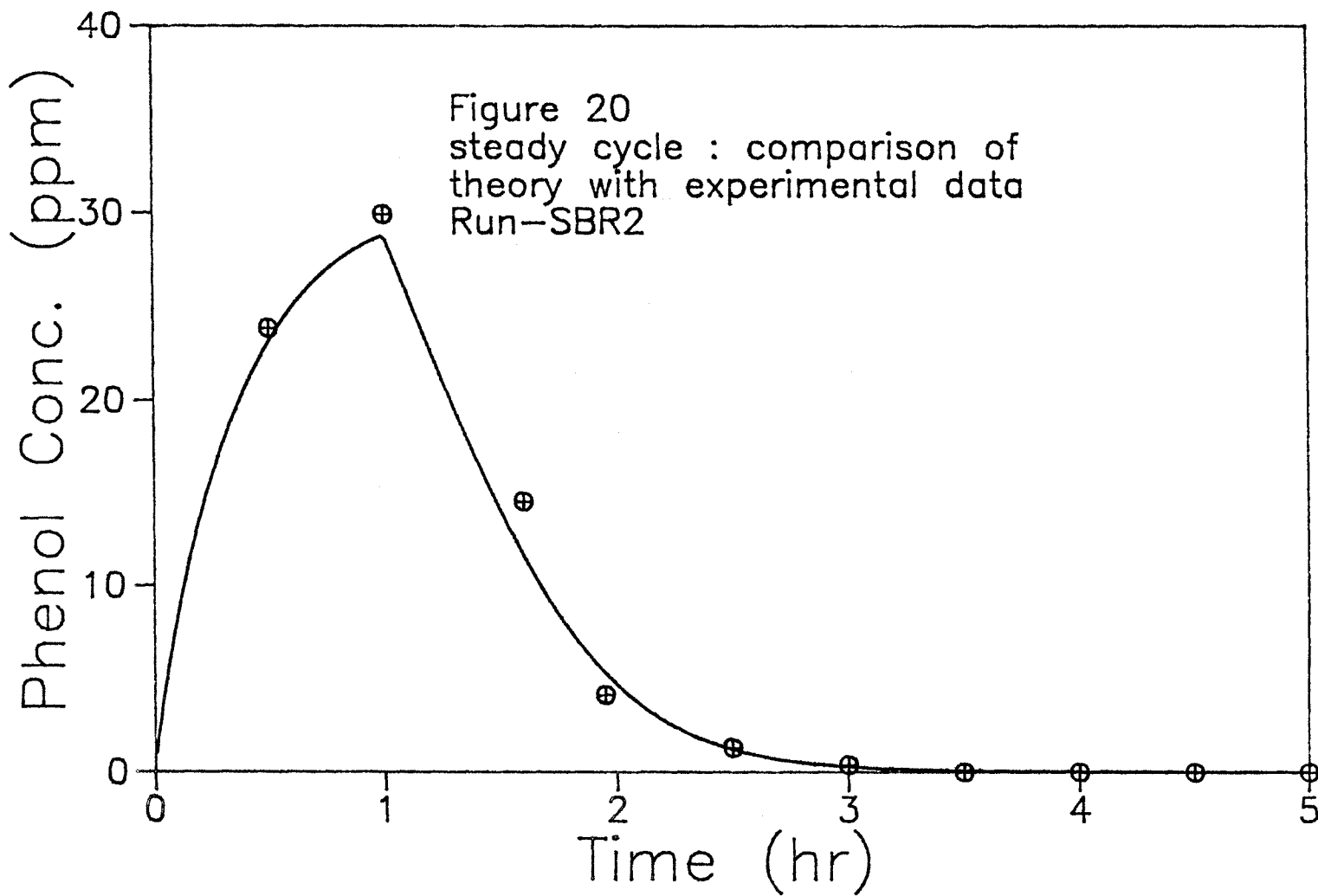


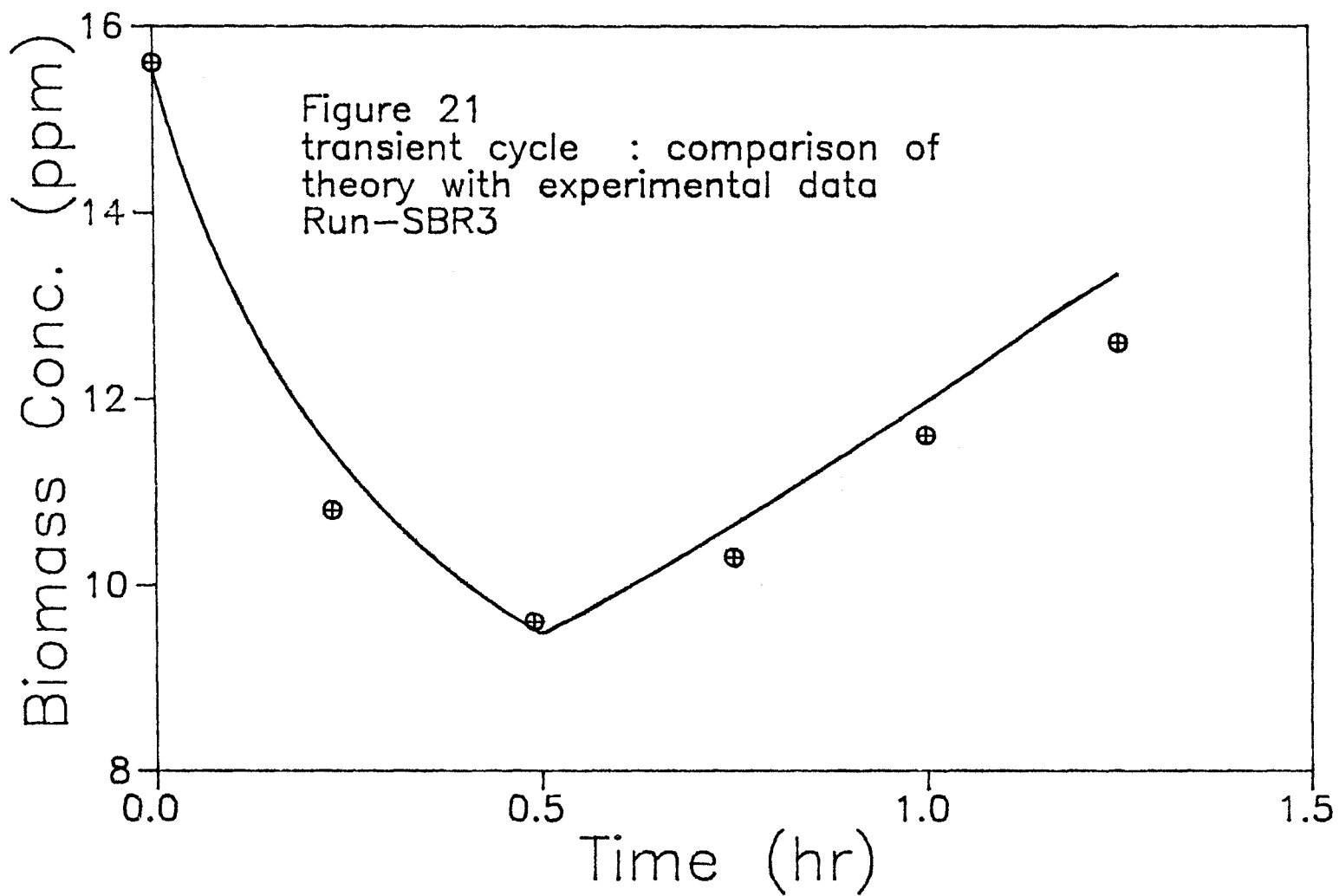


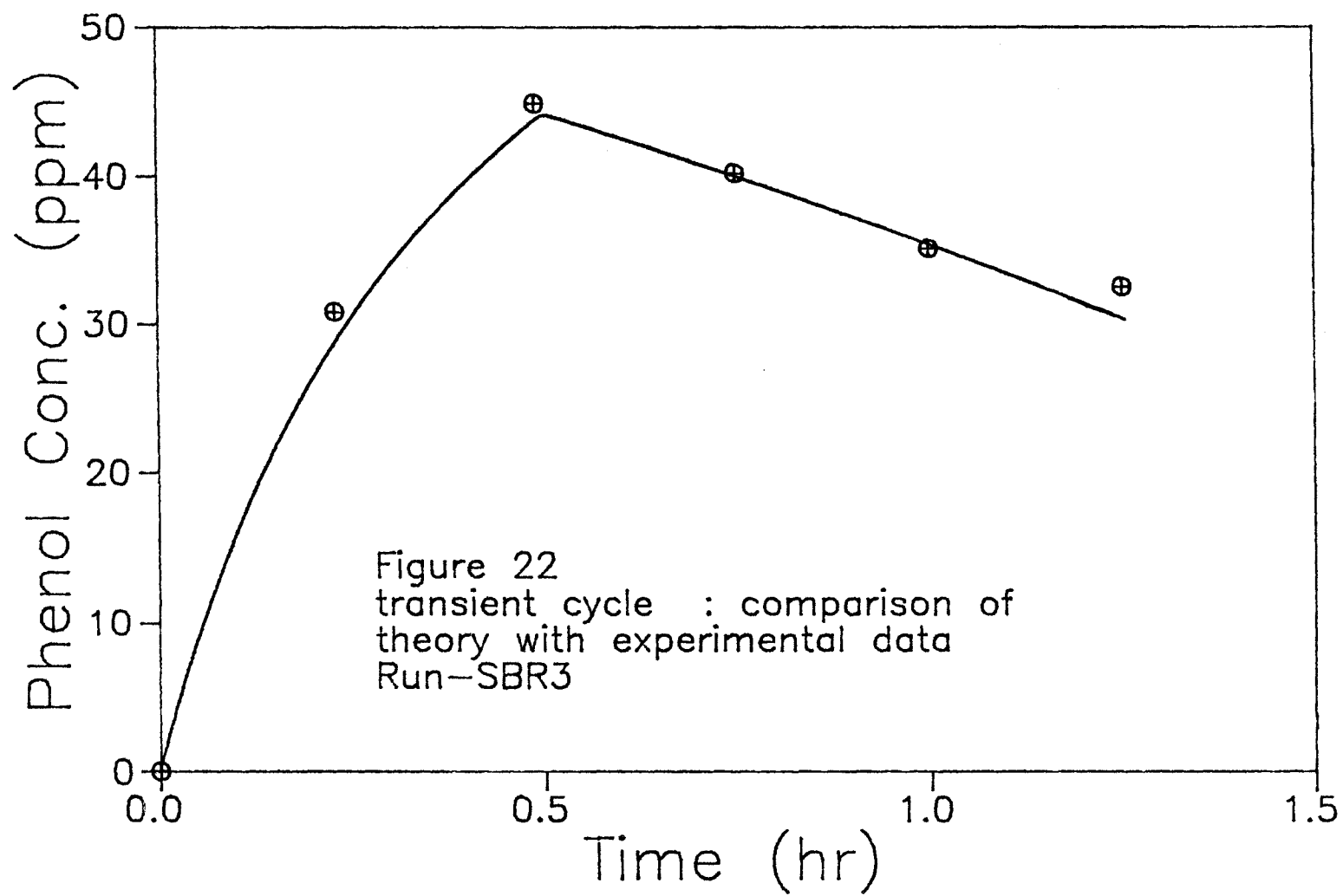


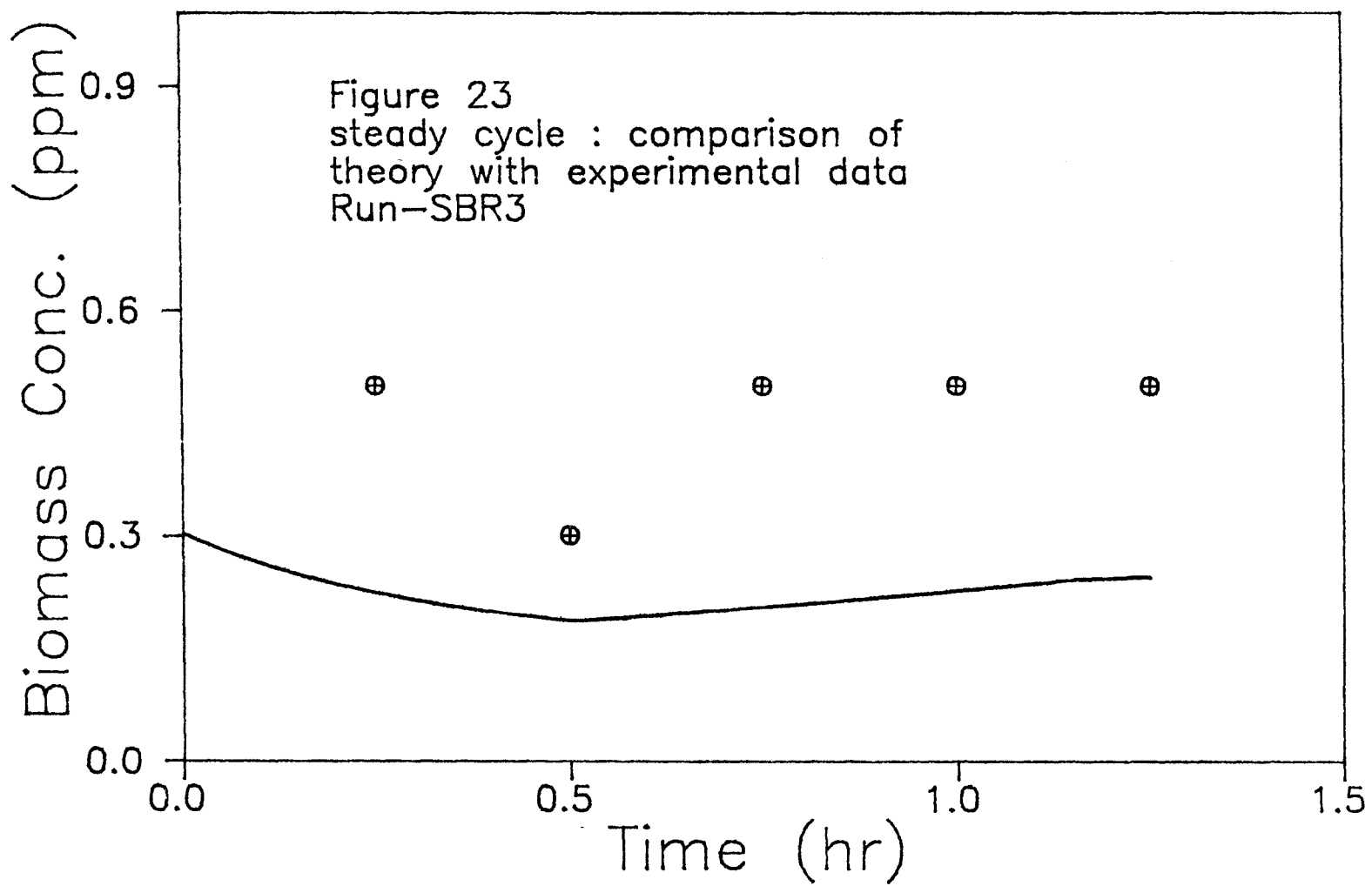


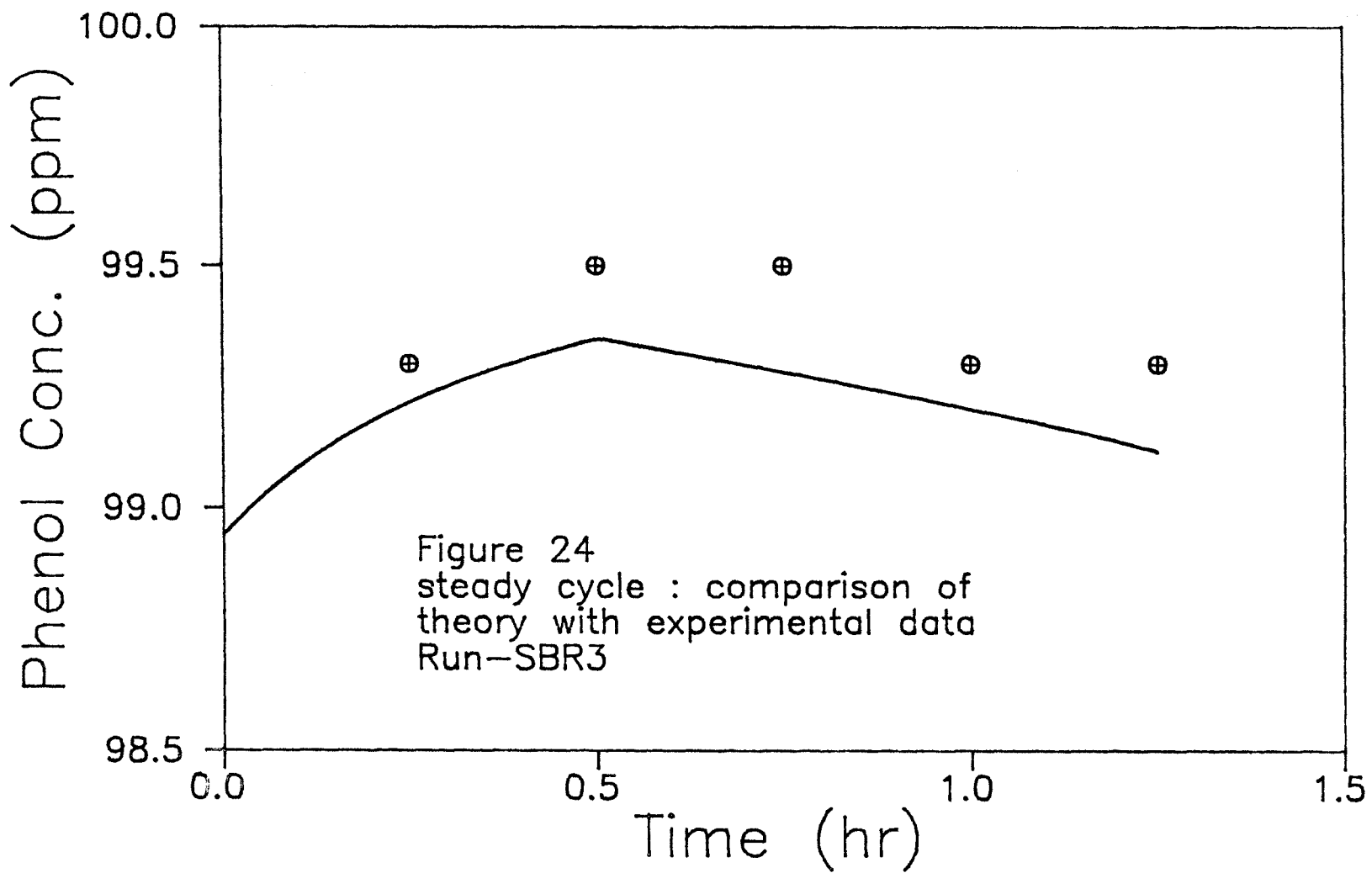


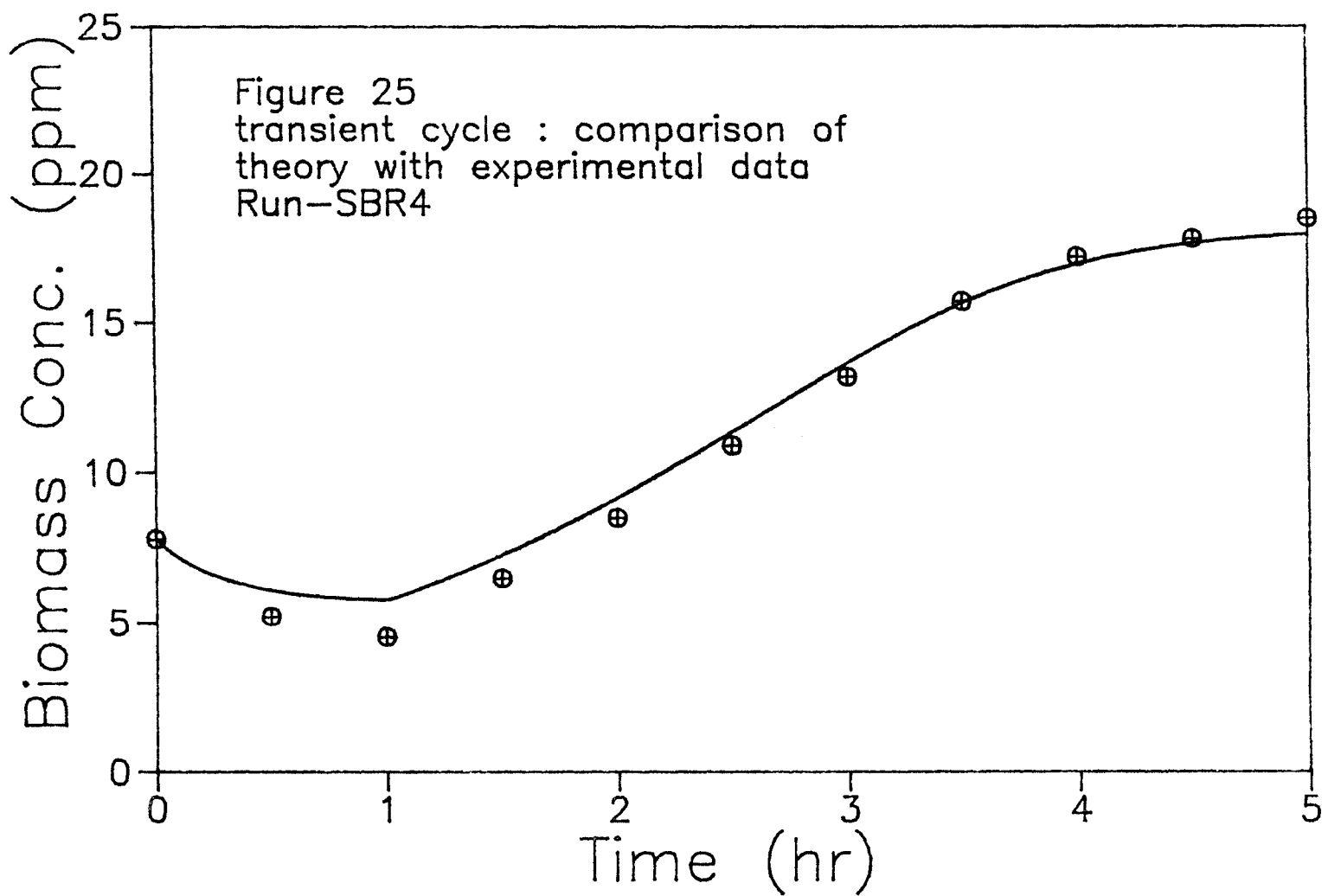


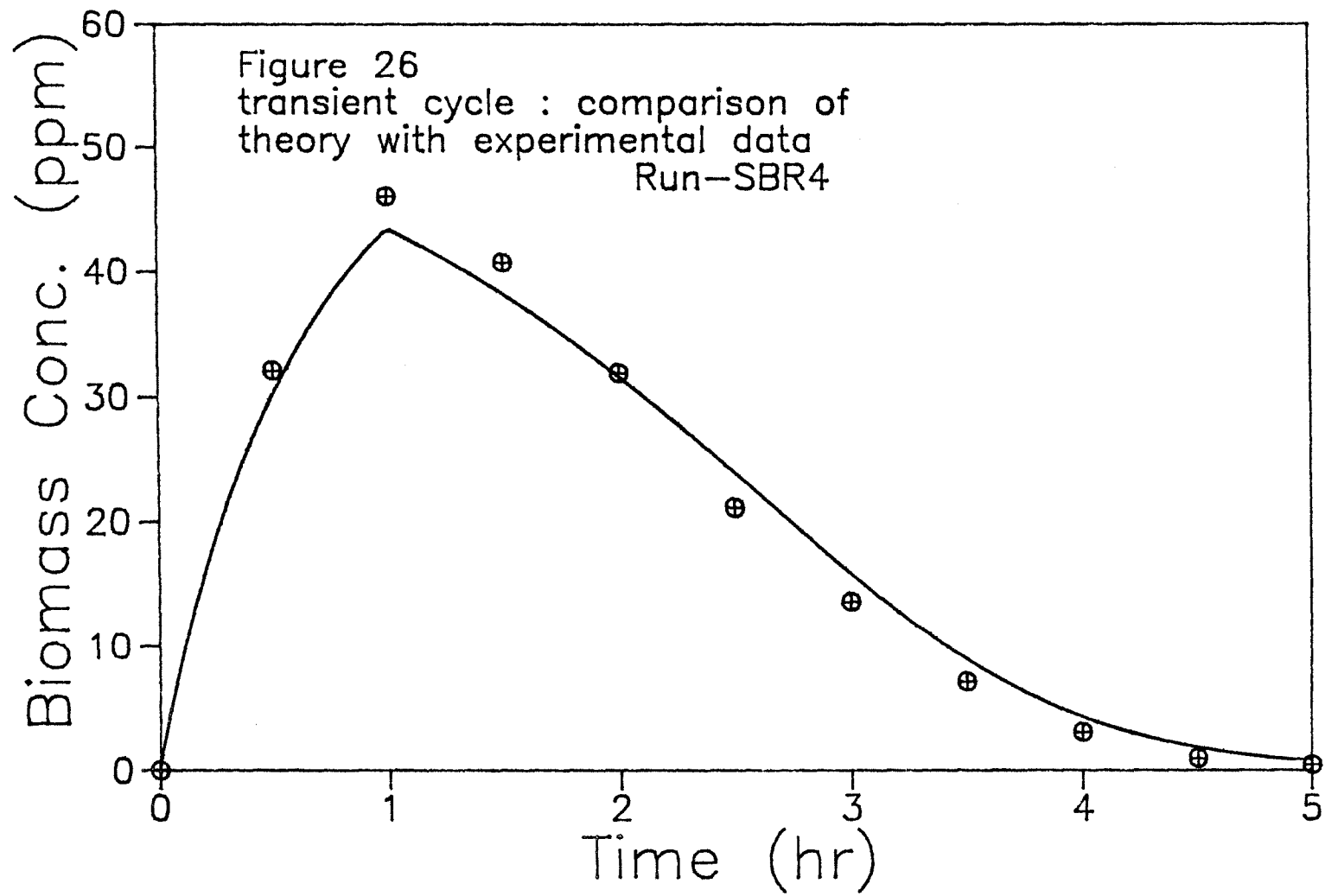


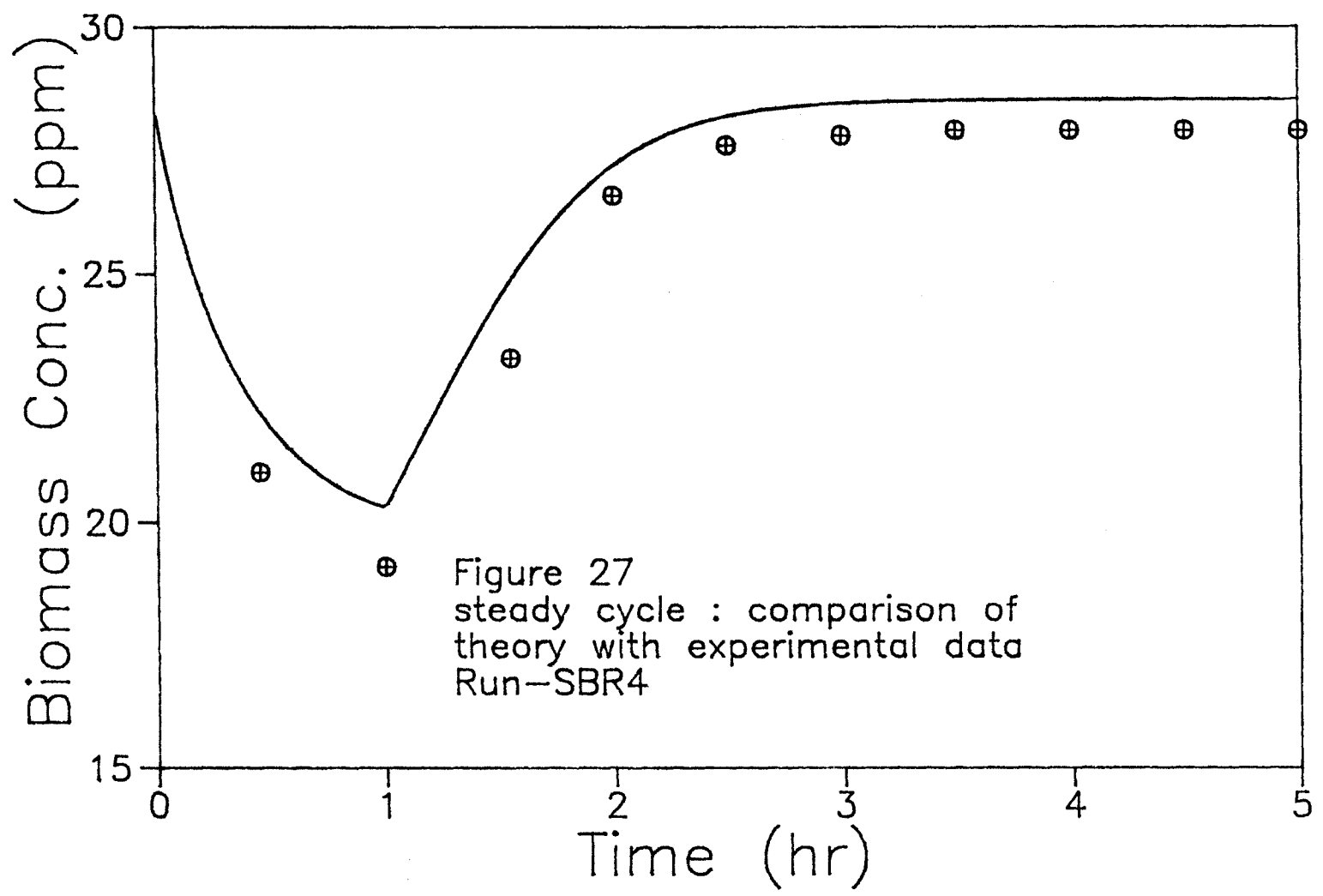


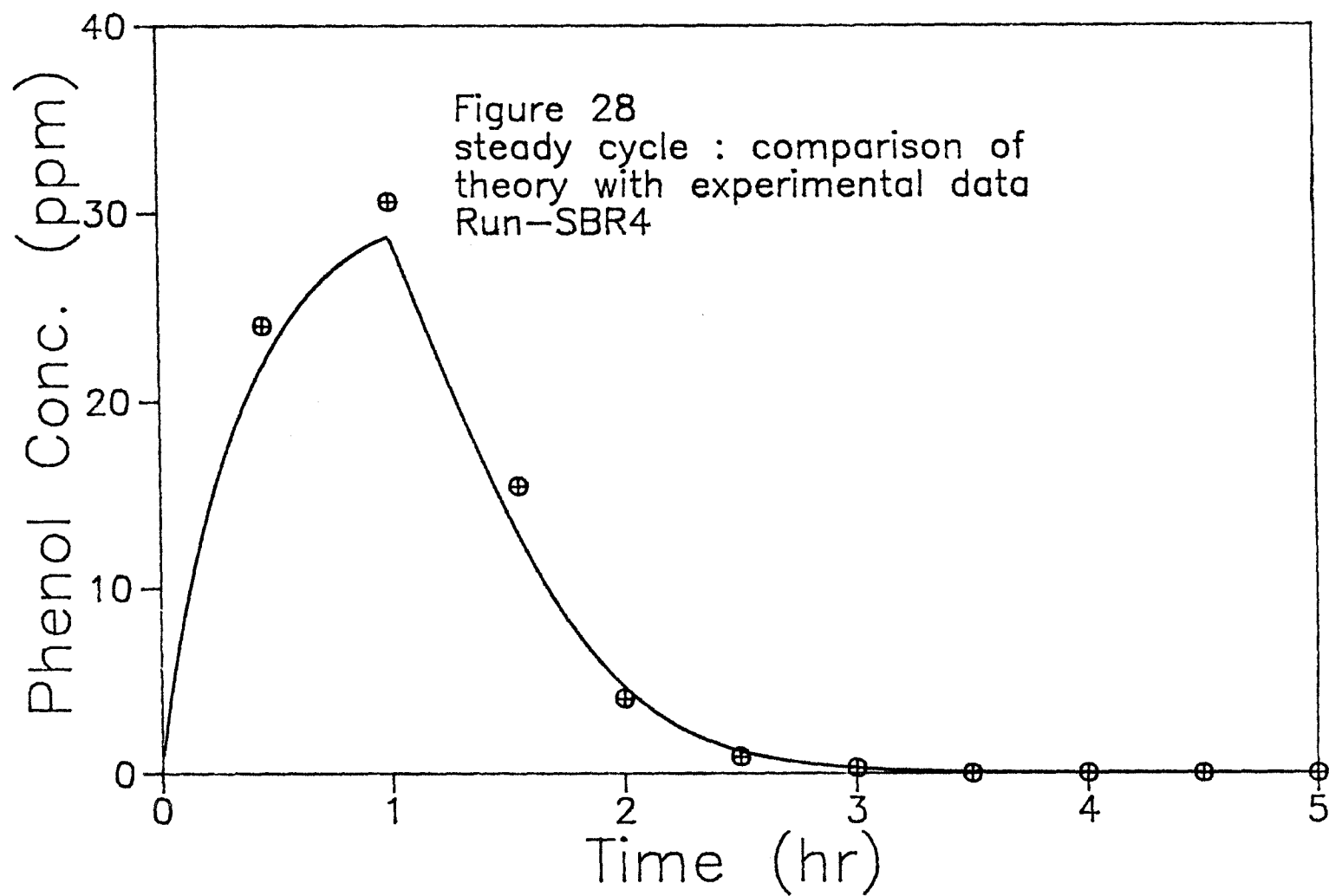


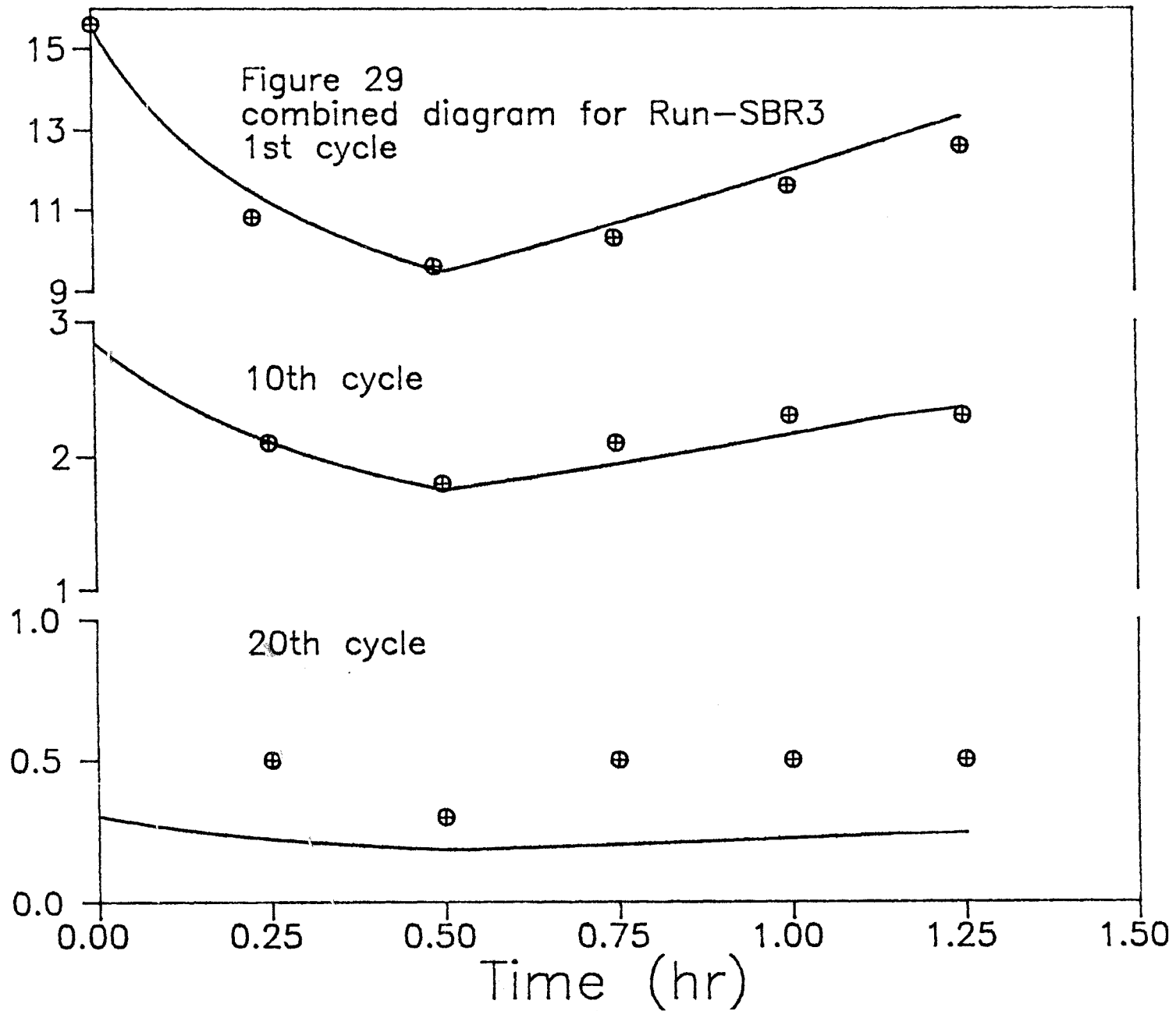


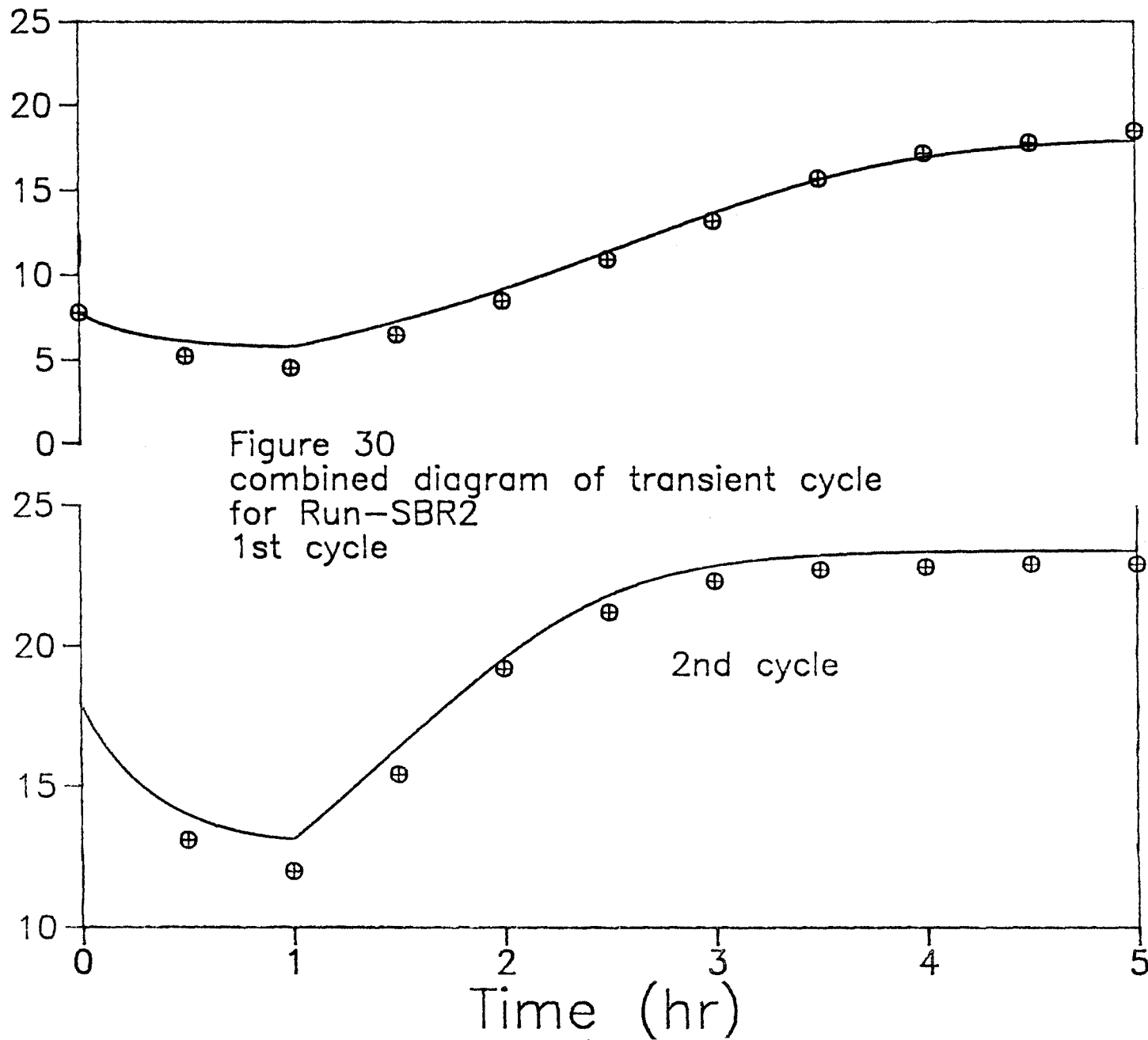


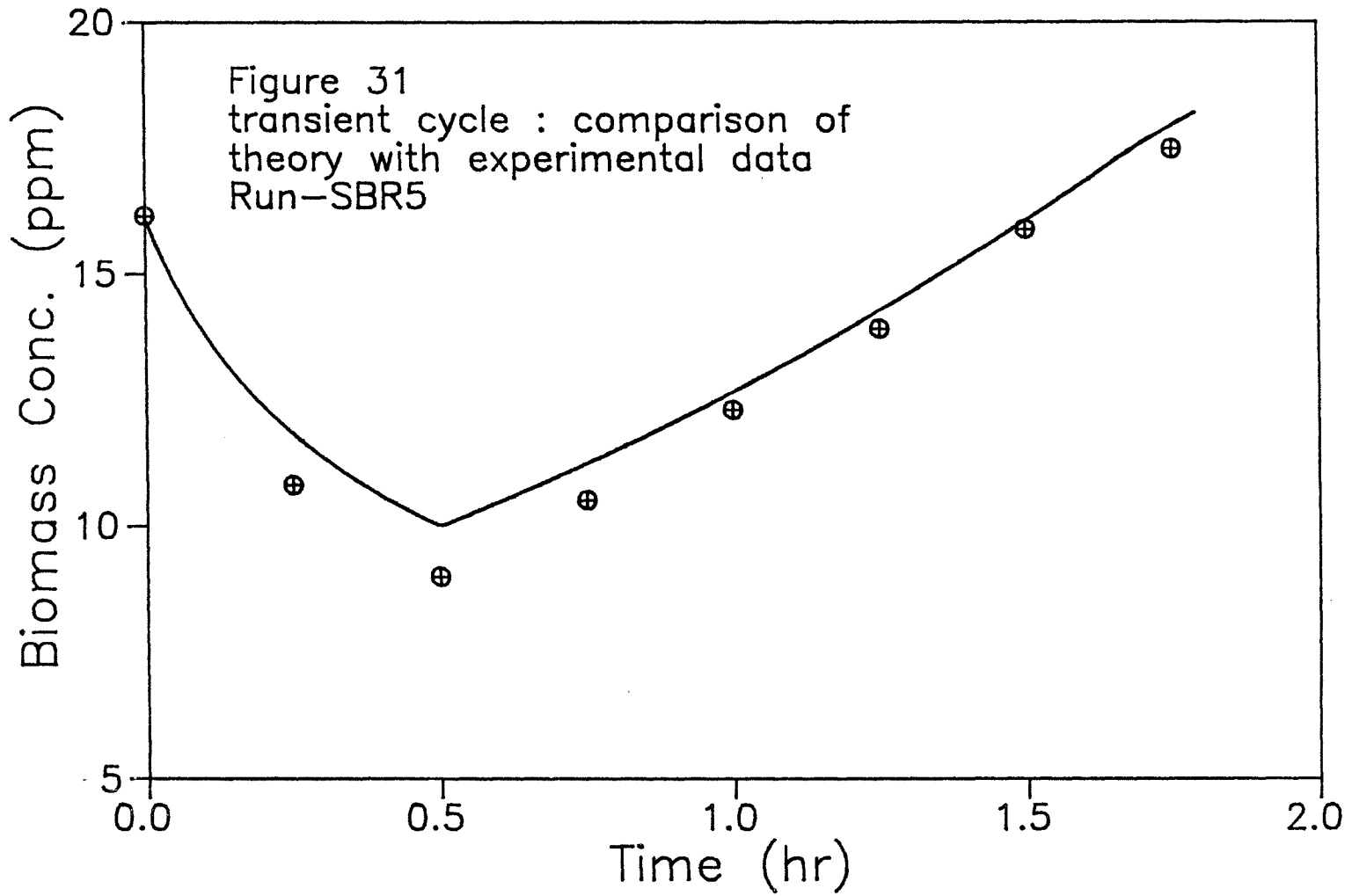


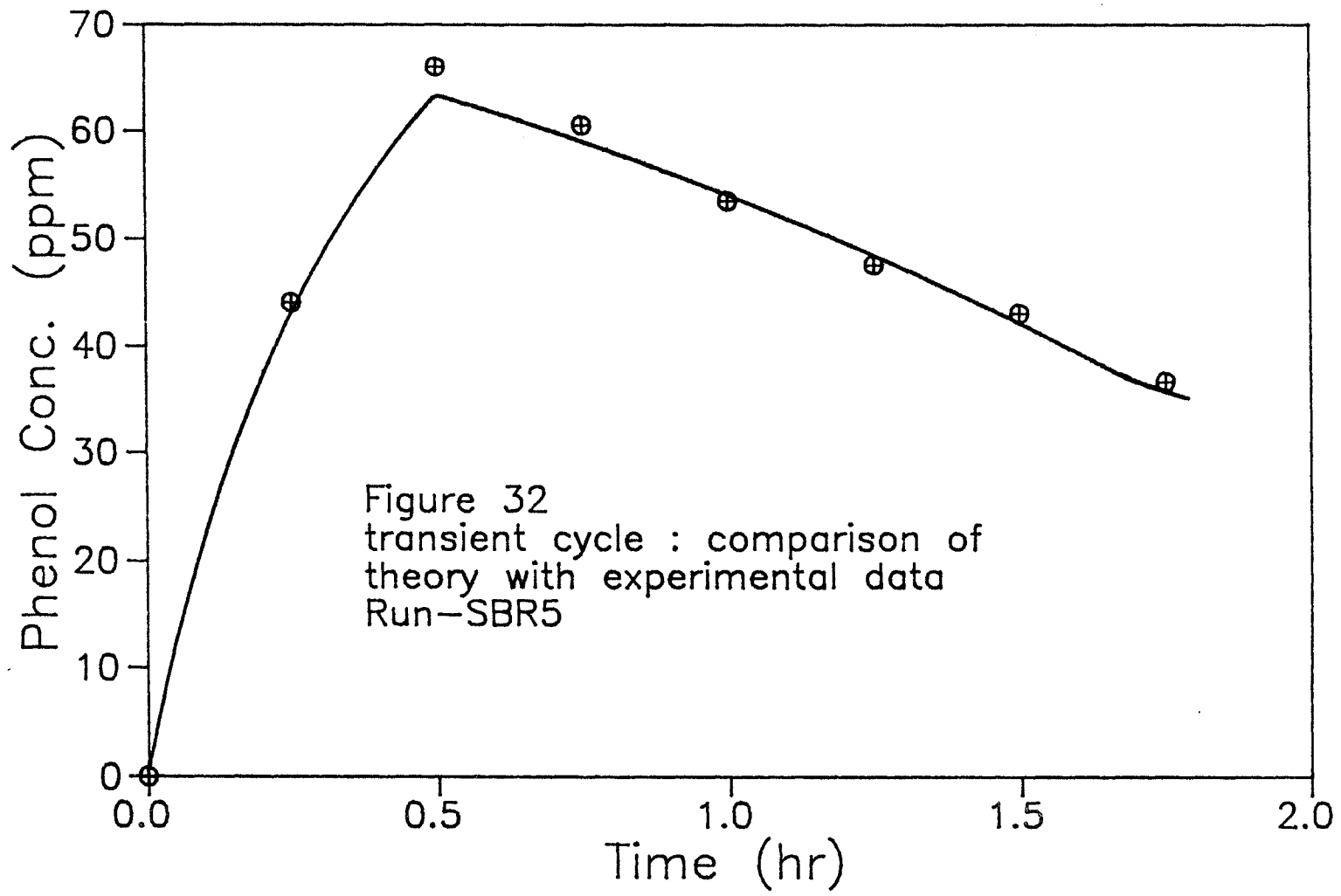


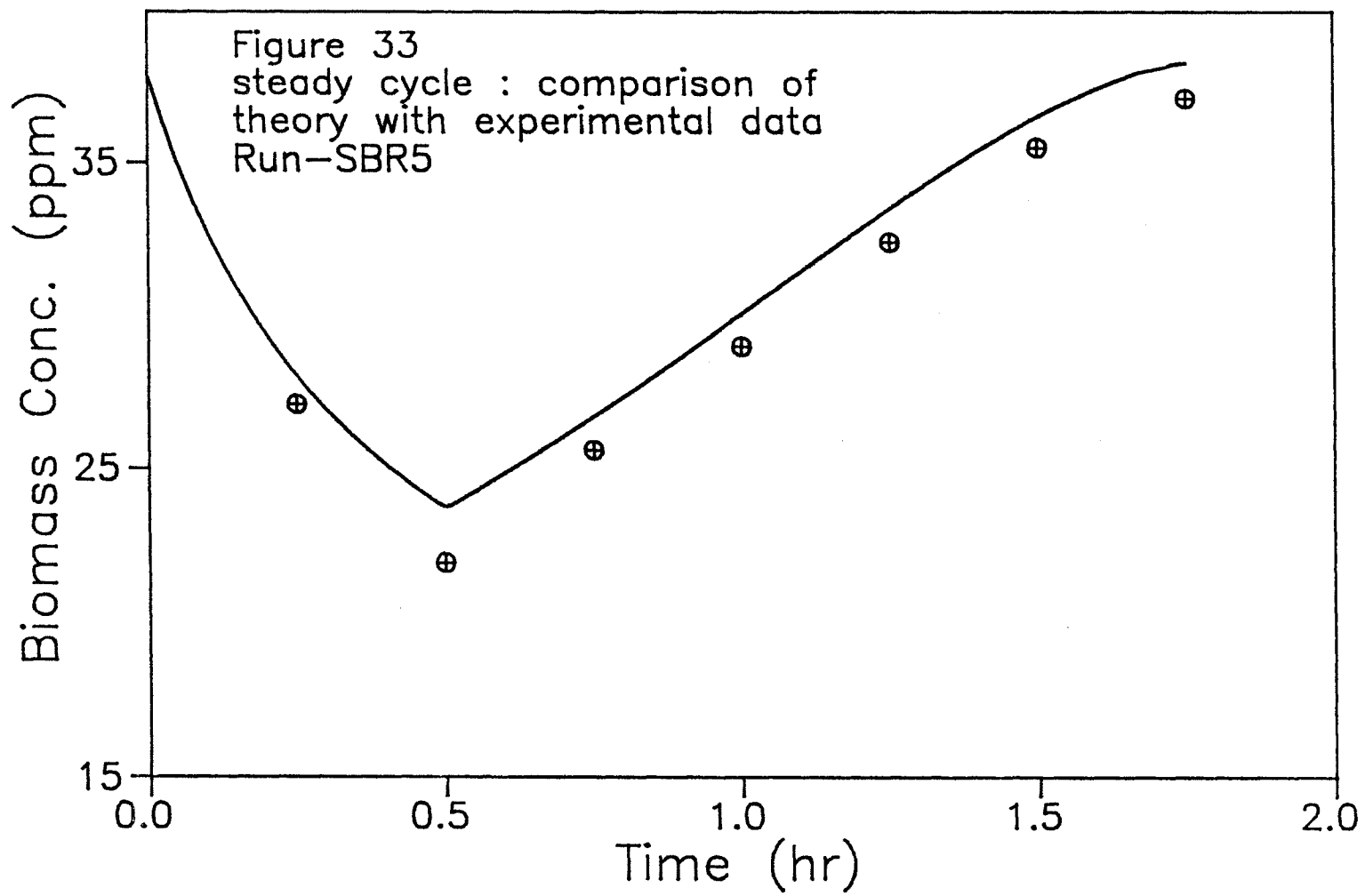


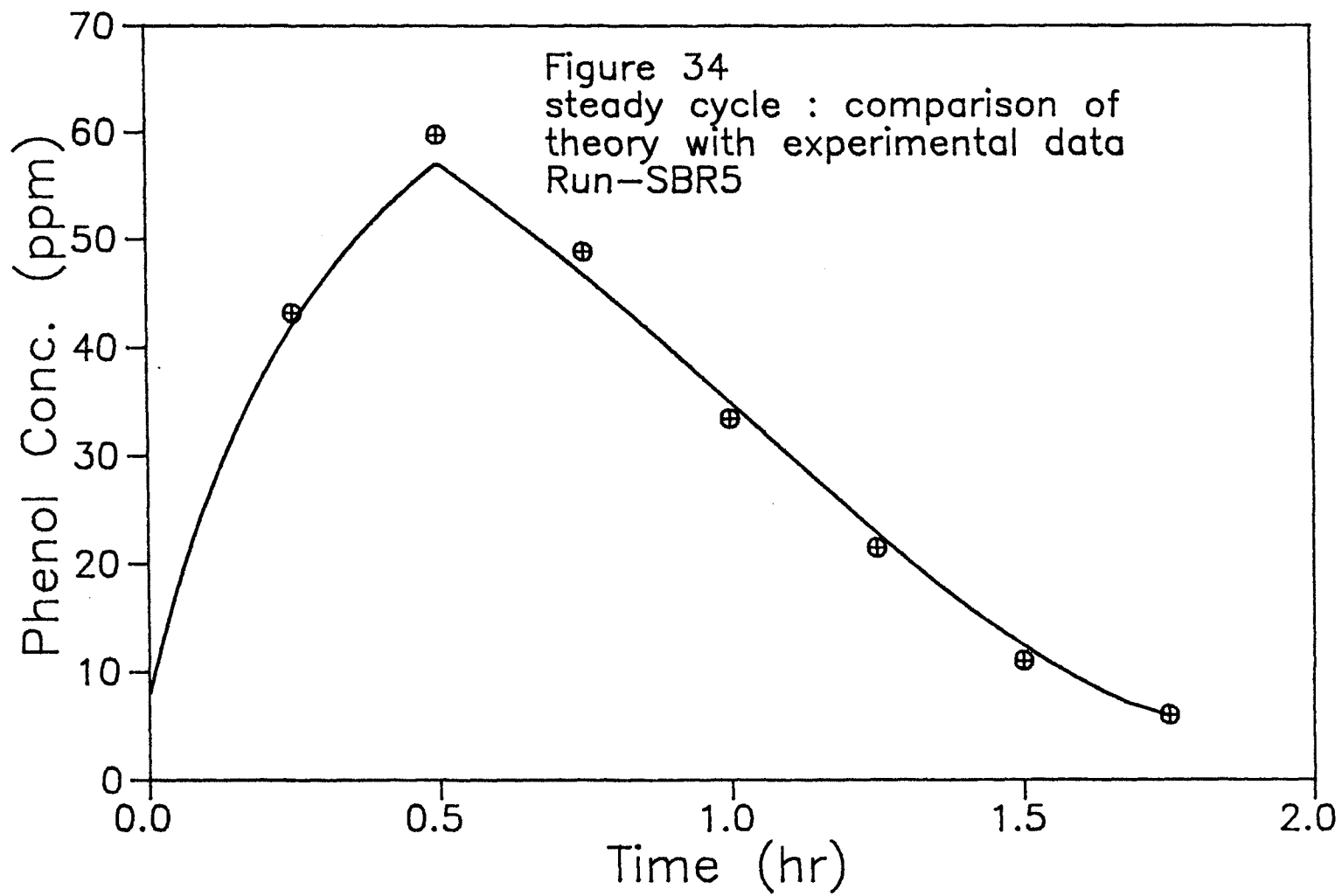


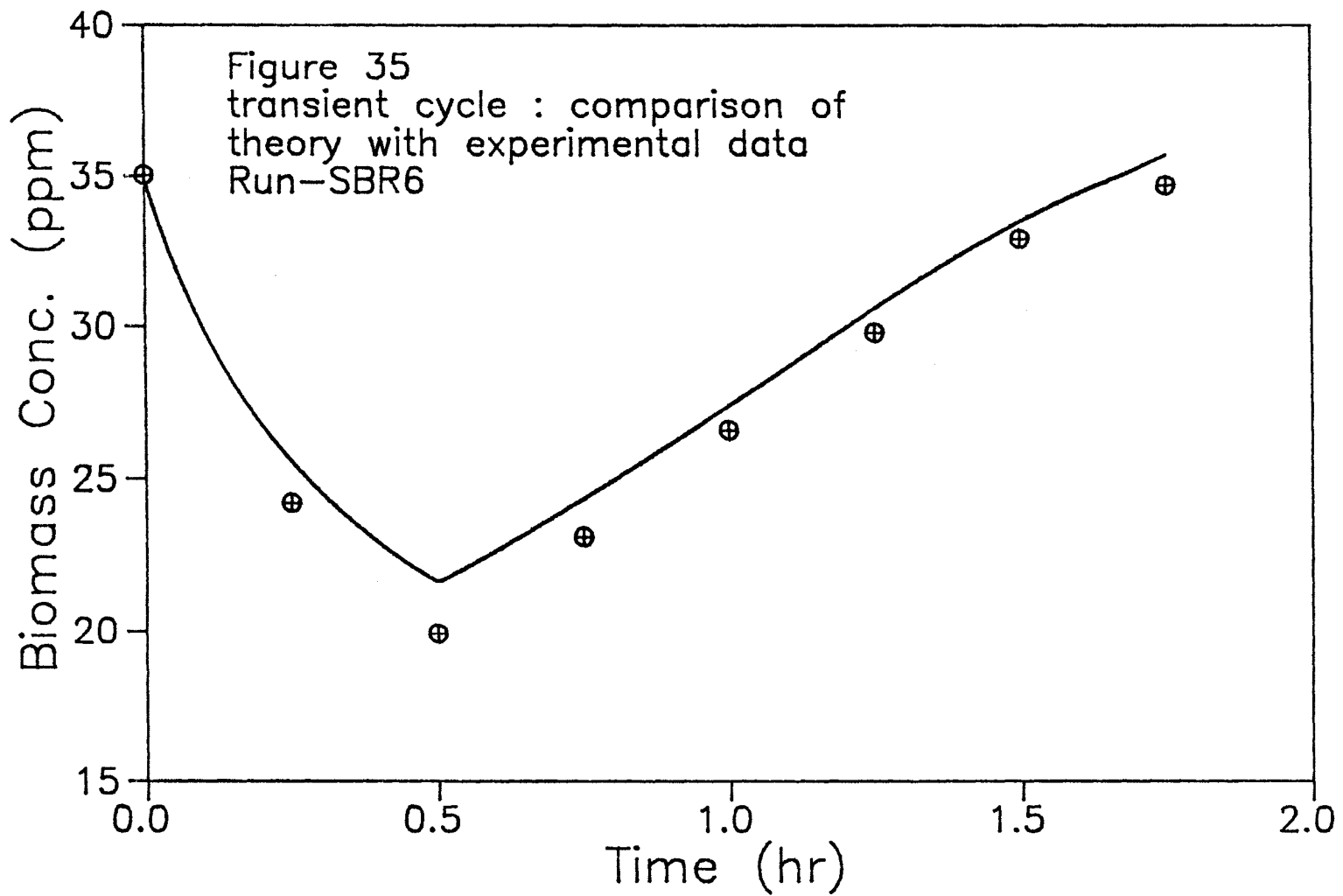


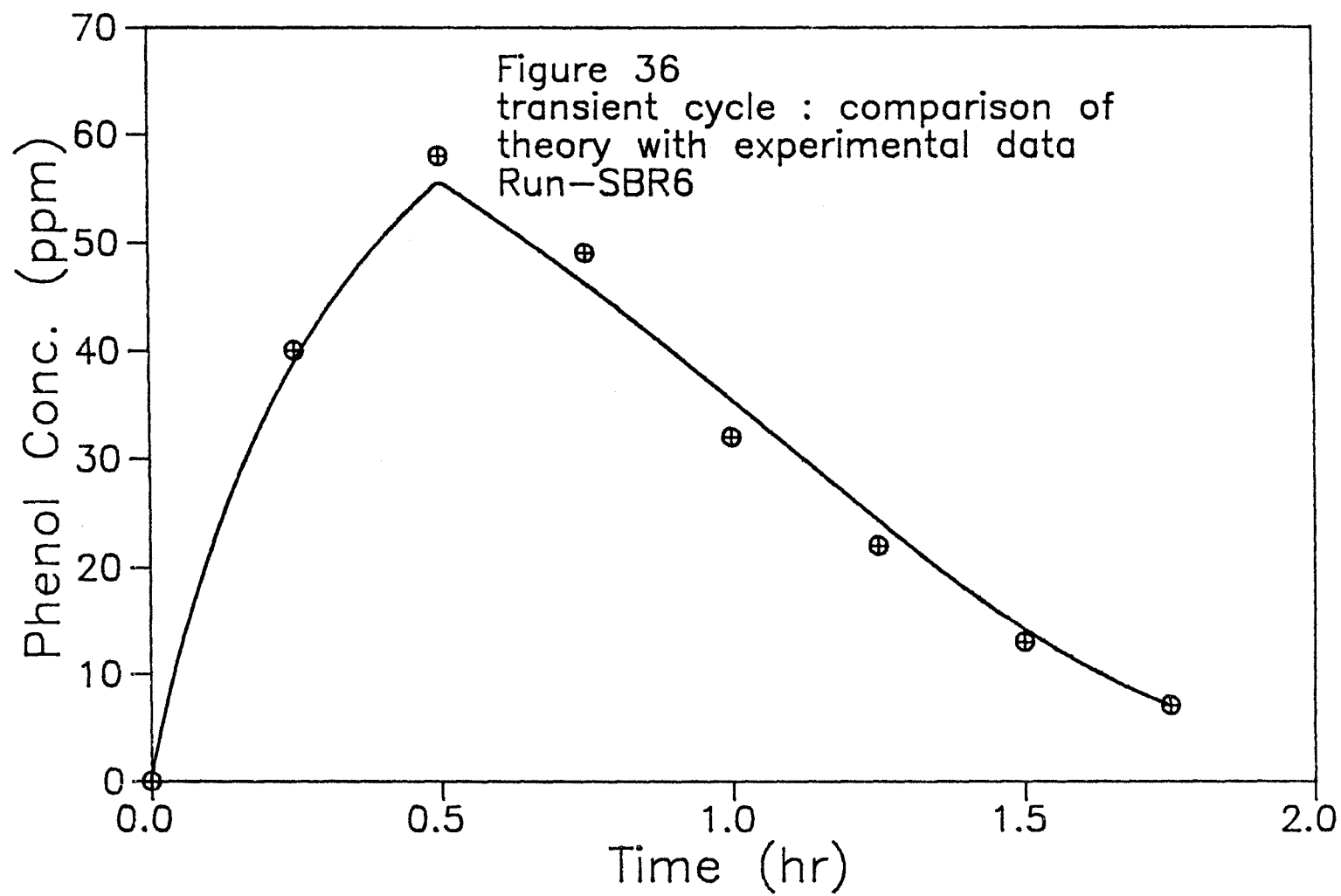


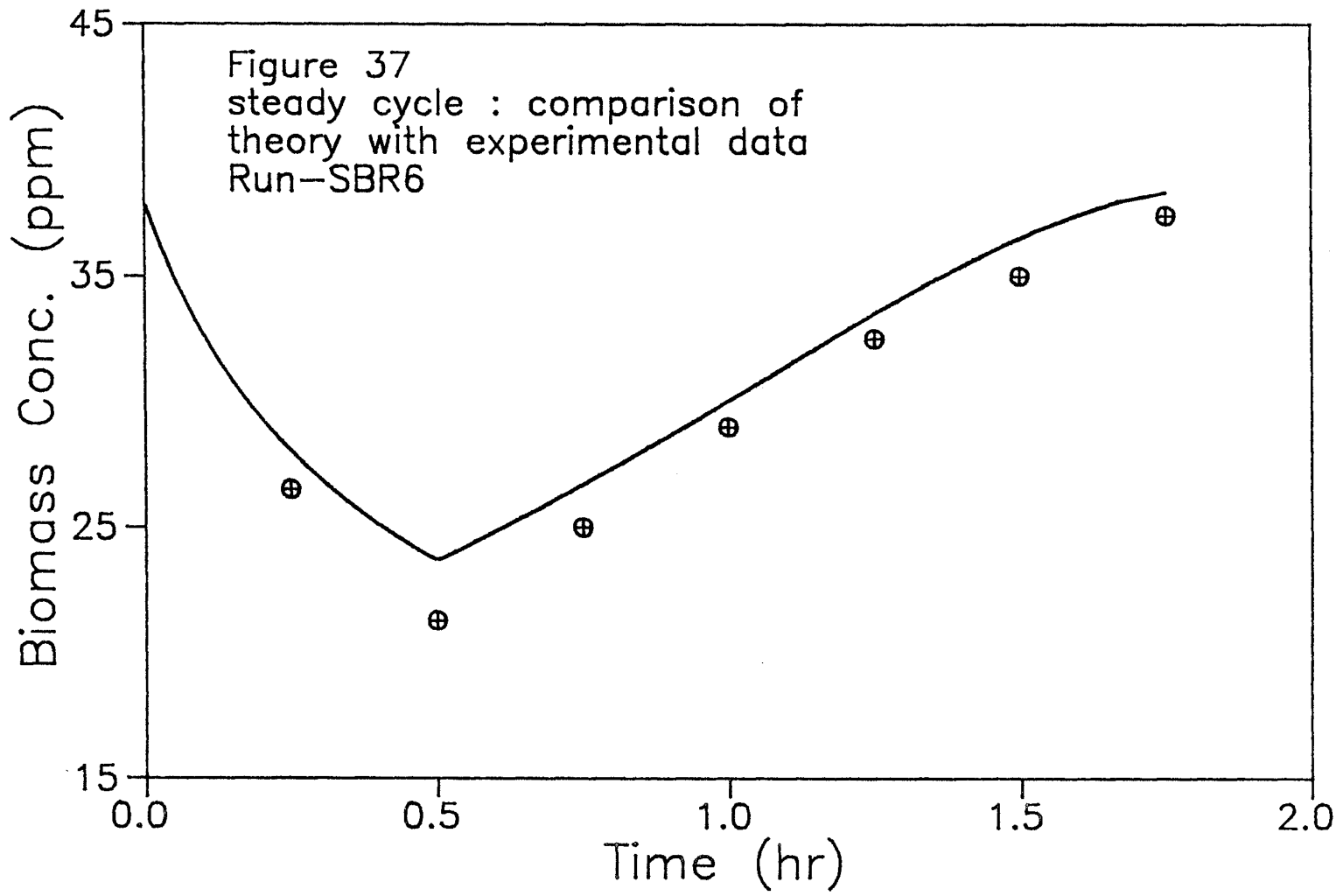


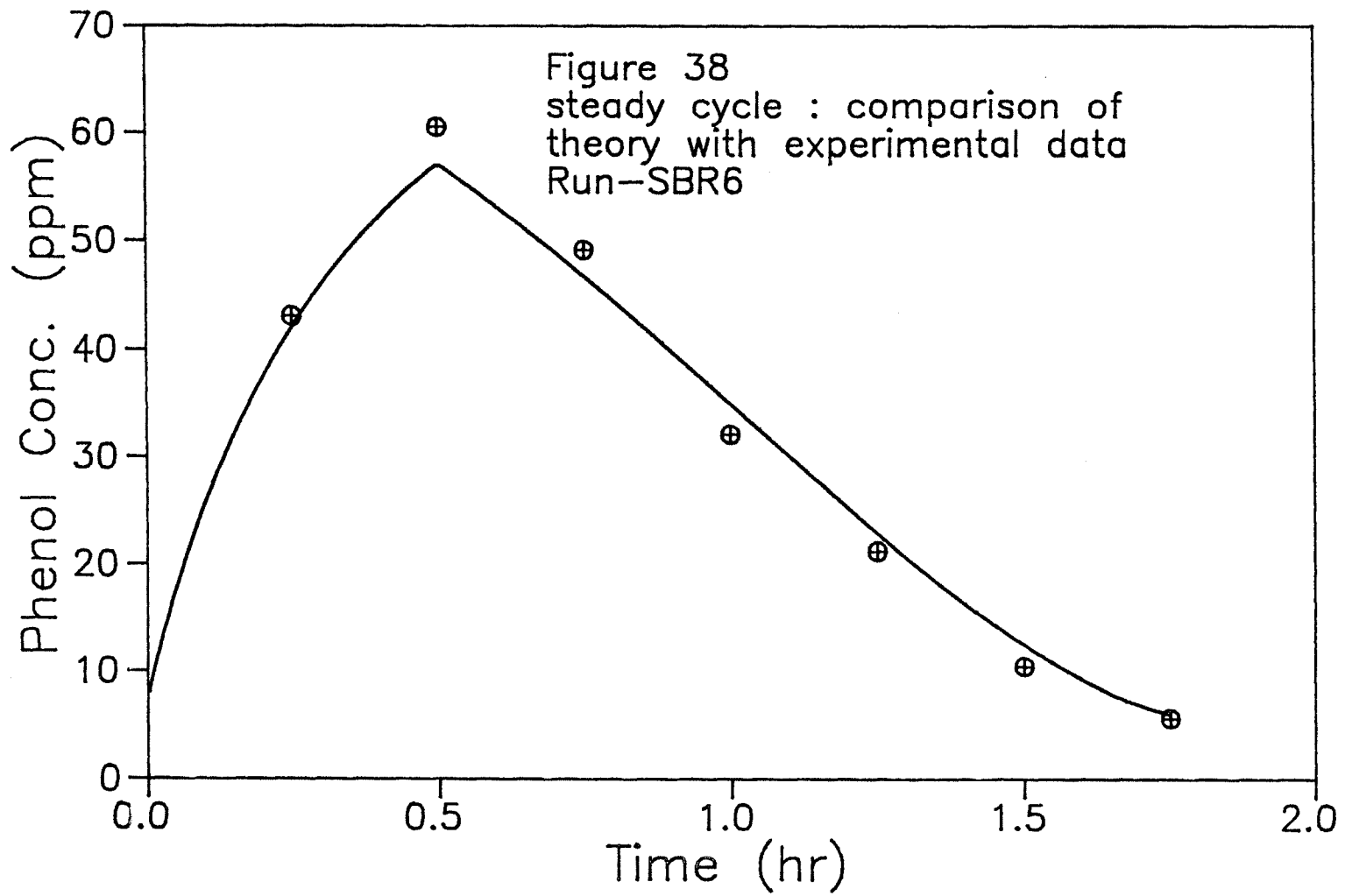












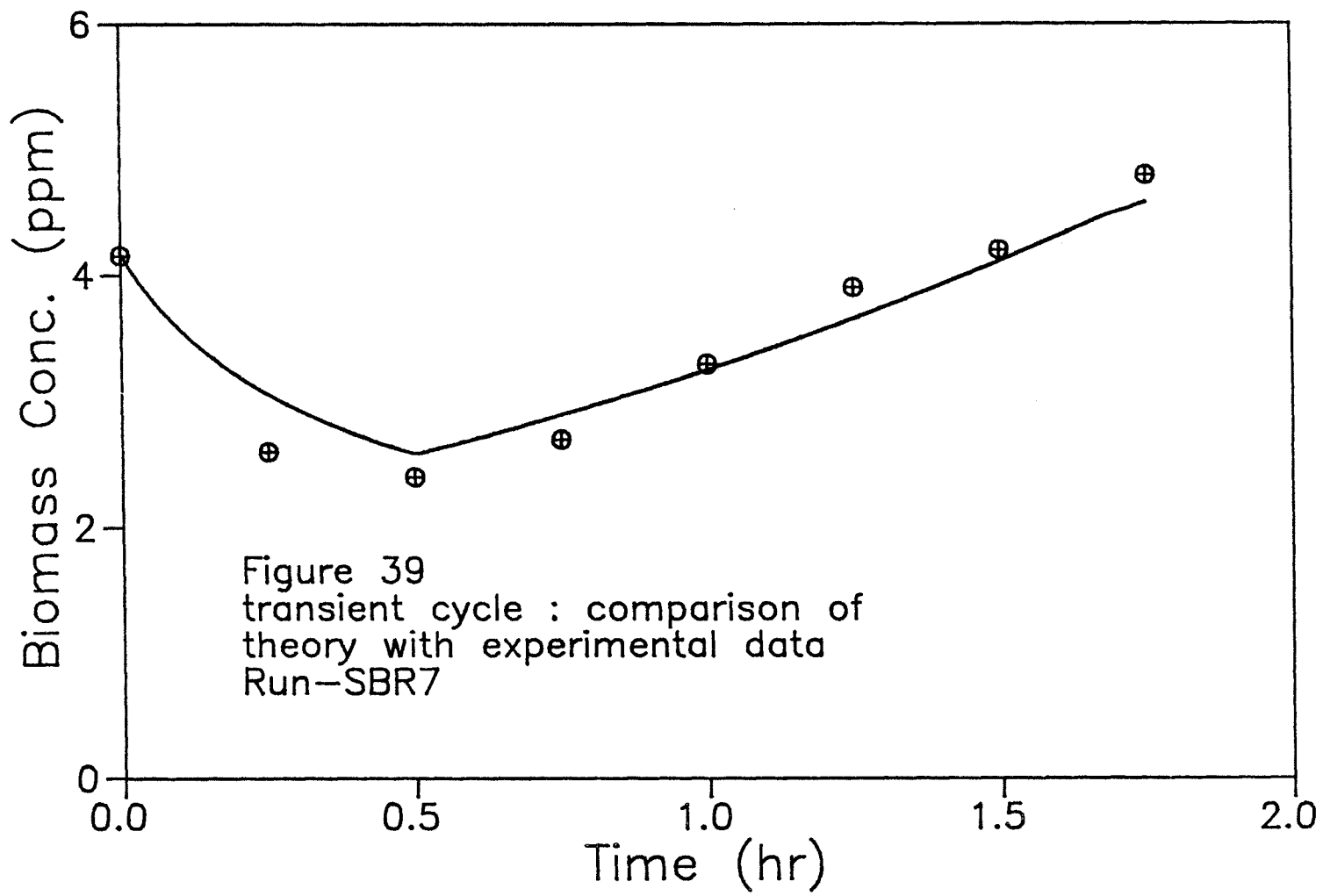
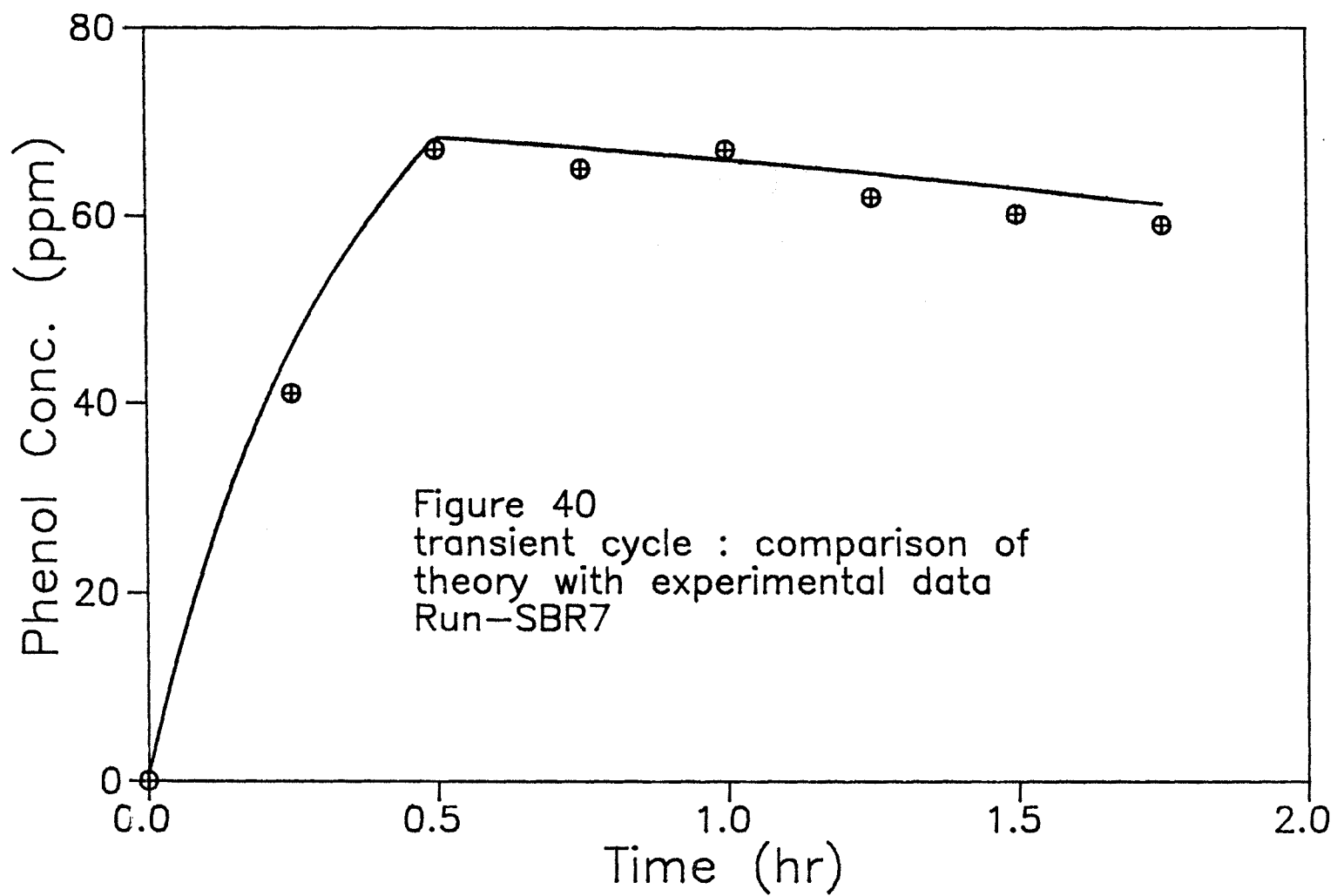
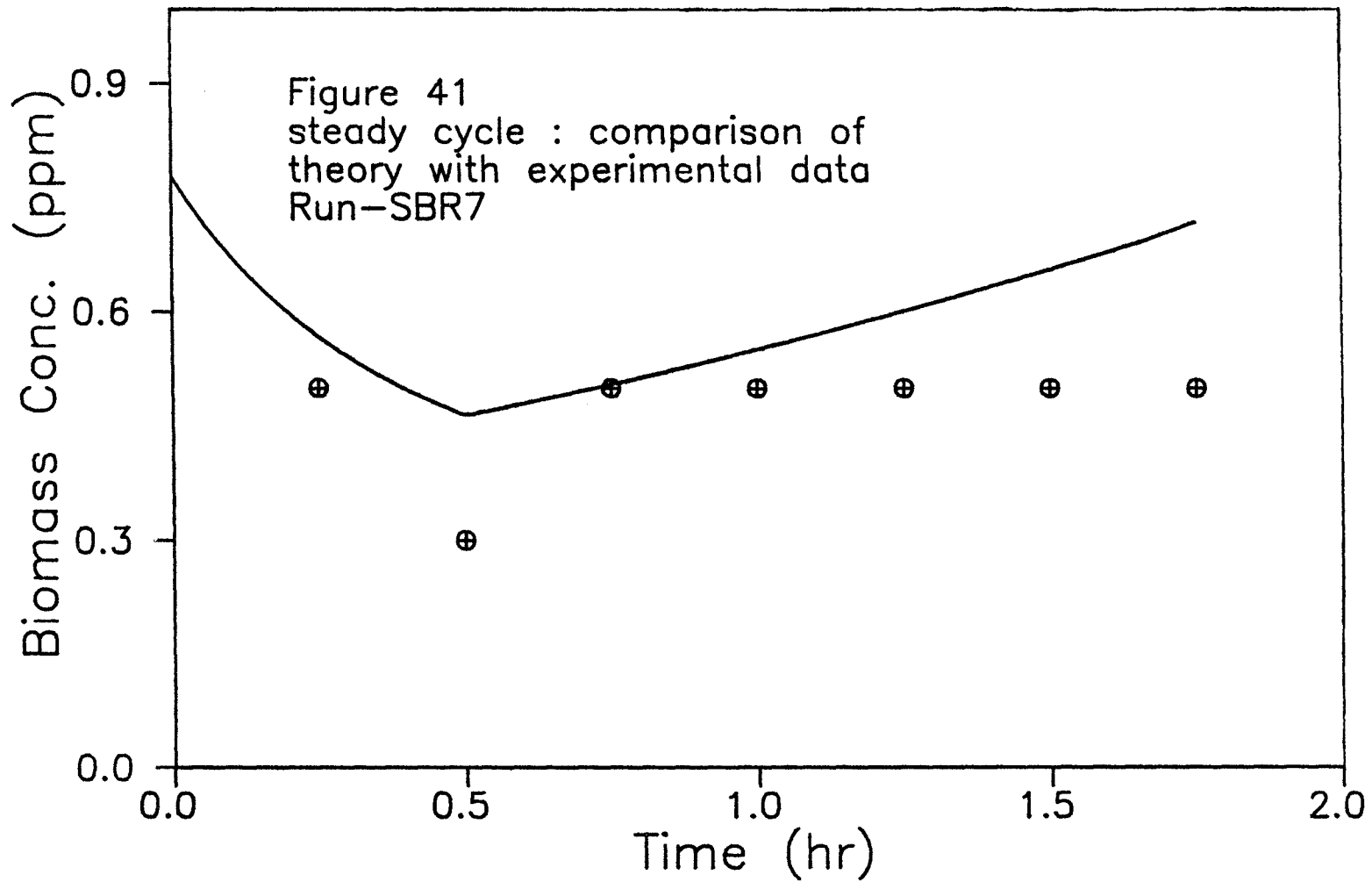
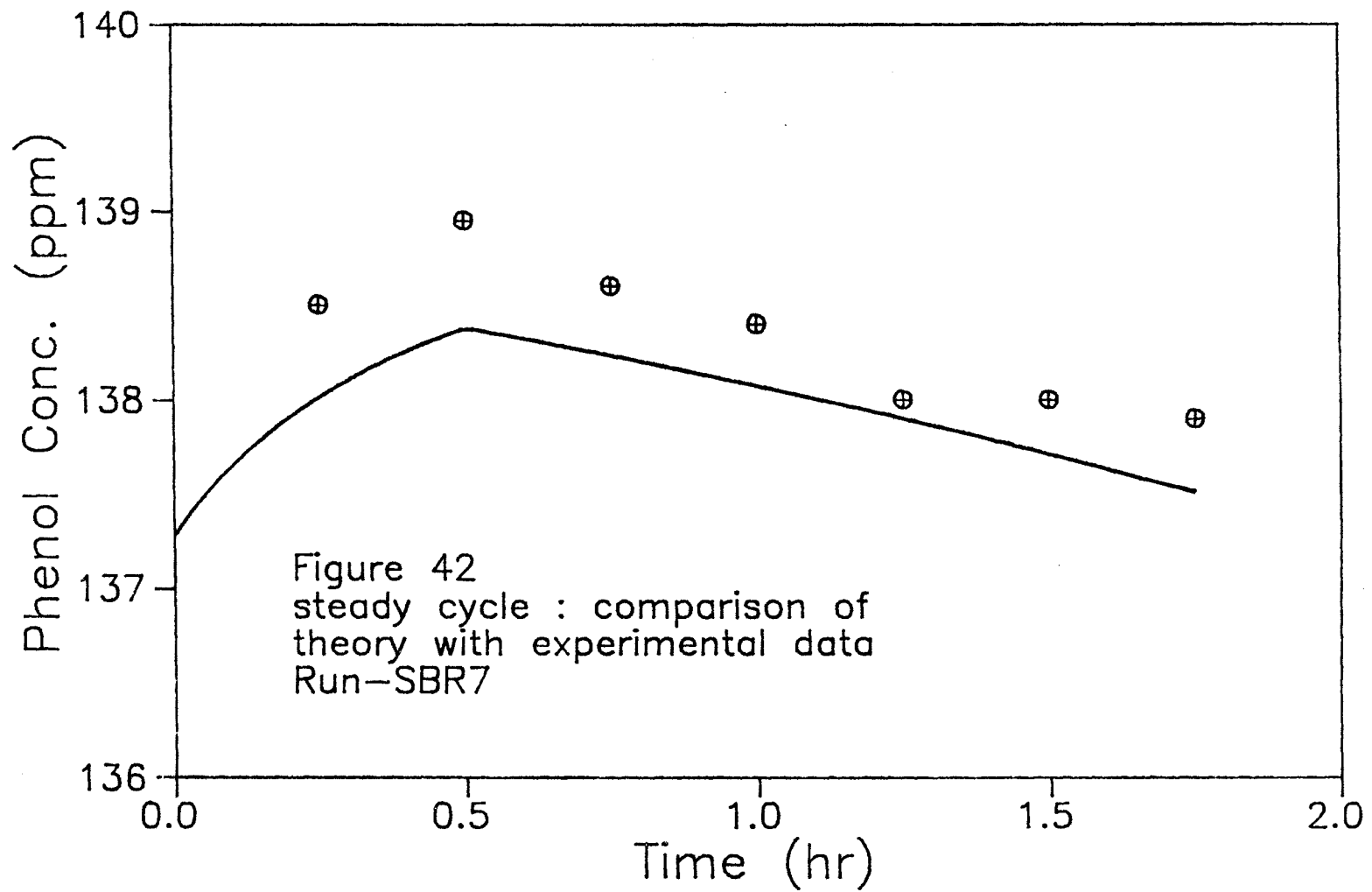


Figure 39
transient cycle : comparison of
theory with experimental data
Run-SBR7







APPFENDIX A
INTORDUCTION TO THE SYSMAC-PO SEQUENCE CONTROLLER

Programming of this sequence controller can be done in the same easy manner as an electronic calculator by merely depressing the appropriate keys in step sequence. SYSMAC-PO automatically shecks key input errors during programming through the keyboard and alerts the operator by a buzzer upon detection of any program error.

Details of programming the sequence controller can be referred to the User's Manual[24]. The following example is the programming procedure used in Run-SBR1 of this study, in which " @ " represents " DEPRESS " followed by the name of a certain key in { } and a brief explanation in ().

- o Turn the "Program Console Switch" to "ON"

- o STEP 1 : (FEED PHASE)
 - * @ { SET STEP }, @ { 0 }, @ { 1 } (set step number " 01 ")

 - * @ { INS }, @ { 9 } (set operation code " 9 ", which is the timer function)

- * @ { 1 }, @ { , } (set value of "DATA-1", which means " 1hr " for fill)
 - * @ { 0 }, @ { 0 },(set value of "DATA-2" which, in conjunction with DATA-1 ,means 1 hr, 0 minute for feed)
 - * @ { OUT } (set output functions)
 - @{ON},{OFF},{OFF},{OFF},{ON},{OFF},{OFF},{OFF}
 - (OUTPUT-1 "ON" means open the feed reservoir solenoid valve. "OUTPUT-5 "ON" means turn on the feed pump)
 - * @ { R/W } (write the set program of STEP 1 into RAM)
- o STEP 2 : (REACT PHASE)
- * { 0 }, @ { 2 } (set step number " 02 ")
 - * @ { INS }, @ { 9 } (same as STEP 1)
 - * @ { 3 }, @ { , } (set "DATA-1" "3hrs")
 - * @ { 5 }, @ { 3 } (set "DATA-2" "53 min" which in conjunction with DATA-1, means 3 hrs, 53 minutes for react)
 - * @ { R/W } (write the set program of STEP 2 into RAM)
- o STEP 3 : (DRAW PHASE)
- * @ { 0 }, @ { 3 }
 - * @ { INS }, @ { 9 }

- * @ { 0 }, @ { 7 }
- * @ { 0 }, @ { 0 }
- * @ { OUT }
- * @ { OFF }, @ { OFF }, @ { OFF }, @ { OFF }, @ { OFF }, @ { OFF }, @ { OFF }, @ { ON }
- (OUTPUT-8 "ON" means open the draw-out solenoid valve)
- * { R/W }

o STEP 4 : (REPEAT THE CYCLE)

- * @ { 0 }, @ { 4 }
- * { INS }, @ { 8 } (set operation code " 8 " ,which is the function of " REPEAT ")
- * @ { 3 }, @ { 0 } (set "DATA-1" which is required for the "REPEAT" function. "30" means repeat the cycle 30 times which was more than enough for one experiment)
- * @ { 0 }, @ { 1 } (set STEP NUMBER [01] to go to)
- * { R/W }

APPENDIX B
COMPUTER PROGRAMS FOR SOLVING
THE MATHEMATICAL MODEL

```
C*****
C
C This program was used to get the Andrews parameters *
C
C*****
```

```
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      DIMENSION XOLD(3),XINC(3),A(4,4)
      OPEN(6,FILE='WW2.OUT',STATUS='NEW')
      DATA ITMAX,N,IPRINT,EPS1,EPS2/50,3,3,0.5E-06
&,0.1E-09/
      XOLD(1)=1.4
      XOLD(2)=47.5
      XOLD(3)=50.99
      CALL NEWTON(ITMAX,N,IPRINT,EPS1,EPS2,XOLD)
      STOP
      END
```

```
C
C
C
```

```
      SUBROUTINE CALCN(GU,A,N)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION GU(3),A(4,4),S(6),U(6),GA(6)
      DATA S(1),S(2),S(3),S(4),S(5),S(6)/20.,60.
&,100.,140.,180.,220./
      DATA U(1),U(2),U(3)/0.373,0.472,0.399/
      DATA U(4),U(5),U(6)/0.348,0.302,0.243/
      DO 15 I=1,6
      GA(I)=GU(2)+S(I)+(S(I)*S(I)/GU(3))
15  CONTINUE
      A(1,1)=0.
      A(1,2)=0.
      A(1,3)=0.
      A(1,4)=0.
      A(2,1)=0.
      A(2,2)=0.
```

```

A(2,3)=0.
A(2,4)=0
A(3,1)=0.
A(3,2)=0.
A(3,3)=0.
A(3,4)=0.
DO 10 I=1,6
A(1,1)=A(1,1)+2.*((S(I)/GA(I))**2)
C   WRITE(*,66)GA(I)
C 66  FORMAT(F16.12)
A(1,2)=A(1,2)+(2.*S(I)/GA(I)**2)*
+(U(I)-(2.*GU(1)*S(I)/GA(I)))
A(1,3)=A(1,3)+(2.*S(I)**3/(GU(3)*
+GA(I))**2)*((GU(1)*S(I)/GA(I))-U(I))
A(1,4)=A(1,4)+(2.*S(I)/GA(I))*(U(I)-
+(GU(1)*S(I)/GA(I)))
A(2,1)=A(2,1)+(2.*S(I)/GA(I)**2)*
+(U(I)-(2.*GU(1)*S(I)/GA(I)))
A(2,2)=A(2,2)+(2.*GU(1)*S(I)/
+GA(I)**3)*((3.*GU(1)*S(I)/GA(I))-2.*U(I))
A(2,3)=A(2,3)+(2.*GU(1)*S(I)**3/(GU(3)**2*
+GA(I)**3))*(2.*U(I)-(3.*GU(1)*S(I)*S(I)/GA(I)))
A(2,4)=A(2,4)+(2.*GU(1)*S(I)/GA(I)**2)
+((GU(1)*S(I)/GA(I))-U(I))
A(3,1)=A(3,1)+(2.*S(I)**3/(GU(3)
+*GA(I))**2)*((GU(1)*S(I)/GA(I))-U(I))
A(3,2)=A(3,2)+(2.*S(I)**3*GU(1)/(GU(3)**2
+*GA(I)**3))*(2.*U(I)-(3.*GU(1)*S(I)/GA(I)))
A(3,3)=A(3,3)+(2.*GU(1)*(S(I)/
+GU(3)*GA(I))**3)*(S(I)*GU(1)*
+((3.*S(I)*S(I)/GU(3)*GA(I))-2.))+
+U(I)*(2.*(GU(2)+S(I))))
A(3,4)=A(3,4)+(2.*GU(1)*S(I)**3
+/(GU(3)*GA(I))**2)*(U(I)-(GU(1)*S(I)/GA(I)))
10  CONTINUE
RETURN
END

```

C
C
C

```

      subroutine newton(itmax,n,iprint,eps1,eps2,xold)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      dimension xold(3),xinc(3),a(4,4)
c      read and print data
C1      read(5,100)itmax,iprint,n,eps1,eps2,
      & (xold(i),i=1,n)
      write(6,200)itmax,iprint,n,eps1,eps2,
      & (xold(i),i=1,n)
c      newton raphson iteration
      do 9 iter=1,itmax
c      call on calcn to set up the a matrix
      call calcn(xold,a,3)
c      call simul to compute jacobian
c      and correction in xinc
      deter=simul(n,a,xinc,eps1,1,4)
      if (deter.ne.0)goto 3
      write(6,201)
C      goto 1
      RETURN
c      check for convergence and update xold value
3      itcon=1
      do 5 i=1,n
      if(abs(xinc(i)).gt.eps2) itcon=0
5      xold(i)=xold(i)+xinc(i)
      if(iprint.eq.1) write(6,202)iter,
      &deter,n,(xold(i),i=1,n)
      if(itcon.eq.0) goto 9
      write(6,203)iter,n,(xold(i),i=1,n)
C      goto 1
      RETURN
9      continue
      write(6,204)
C      goto 1
      RETURN
c      formats for input and output statements
100      format(10x,i3,17x,i1,19x,i3/ 10x,e7.1,
      &13x,e7.1/ (20x,5f10.3))
200      format(10h1itmax = ,i8/ 10h iprint = ,
      &i8/ 10h n = ,i8/ 10h eps1 = ,
      &1pe14.1/ 10h eps2 = ,1pe14.1/
      $ 25h0 xold(1)...xold(,i2,1h)
      &/ 1h / (1h ,1p4e16.6) )
201      format(38h0matrix is ill-conditioned
      & or singular)

```

```

202  format(10h0iter  = ,i8/ 10h deter  = ,e18.5/
    $ 26h          xold(1)...xold(,i2,1h)
    &/ (1h ,1p4e16.6) )
203  format( 23h0successful convergence/ 9h0iter  =,
    $i3/ 26h0          xold(1)...xold(, i2, 1h)
    & / 1h /(1h ,1p4e16.6) )
204  format( 15h0 no convergence )
    end

```

```

c
c
c

```

```

function simul(n,a,x,eps,indic,nrc)
  IMPLICIT DOUBLE PRECISION (A-H,O-Z)
  DIMENSION IROW(50),JCOL(50),JORD(50)
  DIMENSION Y(50),A(NRC,NRC),X(N)

```

```

CCC

```

```

    max=n
    if (indic.ge.0) max=n+1
c    ...is n larger than 50
    if (n.le.50) goto 5
    write(6,200)
    simul=0.0
    return
c    begin elimination procedure
5    deter=1
    do 18 k=1,n
    kml=k-1
c    search for the pivot element
    pivot=0.0
    do 11 i=1,n
    do 11 j=1,n
c    scan irow and jcol array for
c    invalid pivot subscript
    if(k.eq.1) goto 9
    do 8 iscan=1,kml
    do 8 jscan=1,kml
    if (i.eq.irow(iscan)) goto 11
    if (j.eq.jcol(jscan)) goto 11
8    continue
9    if (abs(a(i,j)).le.abs(pivot)) goto 11
    pivot=a(i,j)

```



```

        irow(k)=i
        jcol(k)=j
11      continue
c      insure that selected pivot is larger than eps
        if(abs(pivot).gt.eps) goto 13
        simul=0.0
        return
c      update the determinant value
13     irowk=irow(k)
        jcolk=jcol(k)
        deter=deter*pivot
c      normalize pivot row element
        do 14 j=1,max
14     a(irowk,j)=a(irowk,j)/pivot
c      carry out elimination and develop inverse
        a(irowk,jcolk)=1.0/pivot
        do 18 i=1,n
            aijck=a(i,jcolk)
            if(i.eq.irowk) goto 1
            a(i,jcolk)=-aijck/pivot
        do 17 j=1,max
17     if(j.ne.jcolk) a(i,j)=a(i,j)
        &-aijck*a(irowk,j)
18     continue
c      order solution values (if any)
c      and creat jord array
        do 20 i=1,n
            irowi=irow(i)
            jcoli=jcol(i)
            jord(irowi)=jcoli
20     if (indic.ge.0) x(jcoli)=a(irowi,max)
c      adjust sign of determinant
        intch=0
        nml=n-1
        do 22 i=1,nml
            ip1=i+1
            do 22 j=ip1,n
                if (jord(j).ge.jord(i)) goto 22
                jtemp=jord(j)
                jord(j)=jord(i)
                jord(i)=jtemp
            intch=intch+1
22     continue
        if(intch/2*2.ne.intch) deter=-deter
c      if indic is positive return with results

```

```
        if(indic.le.0)goto 26
        simul=deter
        return
c       if indic is negative or zero
c       ,unscramble the inverse
c       first by rows
26      do 28 j=1,n
        do 27 i=1,n
        irowi=irow(i)
        jcoli=jcol(i)
27      y(jcoli)=a(irowi,j)
        do 28 i=1,n
28      a(i,j)=y(i)
c       then by columns
        do 30 i=1,n
        do 29 j=1,n
        irowj=irow(j)
        jcolj=jcol(j)
29      y(irowj)=a(i,jcolj)
        do 30 j=1,n
30      a(i,j)=y(j)
c       return for indic negative or zero
        simul=deter
        return
c       format for output statement
200    format(10h0n too big )
        end
```

```

C*****
C
C This program was used to solve a set of non-linear
C ordinary differential equations , which describe
C the behavior of an SBR with Andrews kinetics ,by
C applying the 4-th Runge-Kutta method . The
C result were then compared to the experimental data
C
C*****
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION DS(100),DB(100),DT(100)
      OPEN(4,FILE='BST.OUT',STATUS='NEW')

C
C
C
      WRITE(*,2)
      WRITE(4,2)
2      FORMAT(/5X,'***DIMENSIONLESS ANALYSIS
& FOR SBR INHIBITION***'/)
      WRITE(*,4)
      WRITE(4,4)
4      FORMAT(5X,'PARAMETERS FOR INTEGRATING :')
      DATA XF,D,UF,B,GAMA/0.,0.5,2.9723,5.,0.9235/
      DATA H,U0,X0,M/0.001,0.,0.31,100/
      WRITE(*,10)XF,D,UF,B,GAMA
      WRITE(4,10)XF,D,UF,B,GAMA
10     FORMAT(/5X,'XF=',F9.4,5X,'D=',F9.4,5X,
& 'UF=',F6.4,5X,'B=',F9.6,5X,'gama=',f9.6)
      WRITE(*,15)H,U0,X0,M
      WRITE(4,15)H,U0,X0,M
15     FORMAT(/5X,'H=',F9.6,5X,'U(0)=' ,
& F9.4,5X,'X(0)=' ,F9.6,5X,'M=' ,I3)

C
C
      DS(1)=0.
      S1=0.28
      S3=0.065
      WRITE(*,25)S1,S3
      WRITE(4,25)S1,S3
25     FORMAT(/7X,'S1=',F8.5,5X,'S3=',F8.5)
      WRITE(*,27)
      WRITE(4,27)
27     FORMAT(/5X,'TIME',13X,'S',14X,'BIO')

C
      L=0
      N=0
      U=U0

```

```

X=X0
ESB0=0.0
C
DO 80 K=1,55
A=1.0
T=0.00001
30 CALL RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
IF(T.LT.(1.-D)*S1) THEN
IF(K.EQ.15)THEN
T1=3.57143*T
S=47.101*U
BI=13.470886*X
WRITE(*,31)T1,S,BI,K
WRITE(4,31)T1,S,BI,K
31 FORMAT(7X,F9.4,5X,F9.4,5X,F9.4,5X,I2)
ENDIF
GO TO 30
ENDIF
C
A=0.0
40 CALL RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
IF(T.LT.(1.-D)*(1.-S3)) THEN
IF(K.EQ.15)THEN
T2=3.57143*T
S=47.101*U
BI=13.470886*X
WRITE(*,41)T2,S,BI
WRITE(4,41)T2,S,BI
41 FORMAT(7X,F9.4,5X,F9.4,5X,F9.4)
ENDIF
GO TO 40
ENDIF
C
AREA=0.0
P=U
R=T
45 CALL RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
IF(K.EQ.15) THEN
T3=3.57143*T
S=47.101*U
BI=13.470886*X
CCC I=K+1
CCC DT(I)=T3
CC DS(I)=S
CC DB(I)=BI
CC ERROR=DS(I)-DS(K)

```

```

CCCCC 0.0001
CC      IF (ABS(ERROR) .LT. 0.1) THEN
        WRITE(*,46)T3,S,BI,K
        WRITE(4,46)T3,S,BI,K
    46   FORMAT(7X,F9.4,5X,F9.4,5X,F9.4,5X,I3)
        ENDIF
CC      GO TO 90
CC      ENDIF
CC      Y=(P+U)/2.*(T-R)
CC      P=U
CC      R=T
CC      AREA=AREA+Y
CC      IF(T.LT.(1.-D)) THEN
CC      GO TO 45
CC      ENDIF
C
C      ESB=1.-AREA/S3/UF/(1.-D)
C      IF(K.EQ.1) THEN
C      ESB1=ESB
C      ENDIF
C      DV=ESB/ESB1
C      IF(DV.LT.0.01) THEN
C      GO TO 90
C      ENDIF
C      IF(ABS(ESB-ESB0).LT.0.000000000000001) THEN
C      L=L+1
C      IF(L.GT.1) THEN
C      GO TO 90
C      ENDIF
C      ENDIF
C      N=N+1
C      ESB0=ESB
C
    80   CONTINUE
    90   STOP
        END

```

C
C
C
C
C

```

SUBROUTINE RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
IMPLICIT REAL*8 (A-H,O-Z)
F(T,U,X)=A*(UF-U)/(S1*D+T)-X*U*B
& /(1.+U+GAMA*U*U)
G(T,U,X)=A*(XF-X)/(S1*D+T)+X*U*B
& /(1.+U+GAMA*U*U)
DF1=H*F(T,U,X)

```

```
DG1=H*G(T,U,X)
DF2=H*F(T+H/2.,U+DF1/2.,X+DG1/2.)
DG2=H*G(T+H/2.,U+DF1/2.,X+DG1/2.)
DF3=H*F(T+H/2.,U+DF2/2.,X+DG2/2.)
DG3=H*G(T+H/2.,U+DF2/2.,X+DG2/2.)
DF4=H*F(T+H,U+DF3,X+DG3)
DG4=H*G(T+H,U+DF3,X+DG3)
U=U+(DF1+2.*DF2+2.*DF3+DF4)/6.
X=X+(DG1+2.*DG2+2.*DG3+DG4)/6.
T=T+H
RETURN
END
```

```

C*****
C
C   This program was used to solve a set of non-linear
C   ordinary differential equations , which describe
C   the behavior of an SBR with Andrews Kinetics , by
C   applying the 4-th Runge-Kutta method . The
C   results were then used to preare the operating
C   diagram for the SBR system .
C
C*****

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      OPEN(4,FILE='CST3C.OUT',STATUS= 'NEW')

C
C
C
      DATA XF,D,S1,GAMA /0.,0.5,0.0926,0.9235/
      DATA H,U0,X0,M,Z /0.005,0.,10.,100,0.015/
      WRITE(*,10)
      WRITE(4,10)
10     FORMAT(/5X,'***DIMENSIONLESS ANALYSIS FOR
&     SBR-CST INHIBITION***',/)
      WRITE(*,20)
      WRITE(4,20)
20     FORMAT(5X,'PARAMETERS FOR INTEGRATING :')
      WRITE(*,30)XF,D,S1,GAMA
      WRITE(4,30)XF,D,S1,GAMA
30     FORMAT(/5X,'XF=' ,F9.4,5X,'D=' ,F9.4,5X,'S1='
&     ',F8.6,5X,'GAMA=' ,F7.5)
      WRITE(*,40)H,U0,X0,M,Z
      WRITE(4,40)H,U0,X0,M,Z
40     FORMAT(/5X,'H=' ,F9.6,5X,'U(0)=' ,F9.4,5X,
&     'X(0)=' ,F9.4,5X,'M=' ,I3,5X,'Z=' ,F9.4)

C
C
      WRITE(*,50)
      WRITE(4,50)
50     FORMAT(/5X,'UF' ,8X,'1/B' ,9X,'ESB')
      S3=0.0185

C
      DO 150 J=0,10
      UF=1.+0.2*J

```

```

SURV=0.0
WASH=0.0
BI=0.0001
C
60  B=1.0/BI
    U=U0
    X=X0
    ESB0=0.0
C
    DO 100 K=1,M
    A=1.0
    T=0.00001
70  CALL RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
    IF(T.LT.(1.-D)*S1) THEN
    GO TO 70
    ENDIF
C
    A=0.0
80  CALL RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
    IF(T.LT.(1.-D)*(1.-S3)) THEN
    GO TO 80
    ENDIF
C
    AREA=0.0
    P=U
    R=T
90  CALL RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
    Y=(P+U)/2.*(T-R)
    P=U
    R=T
    AREA=AREA+Y
    IF(T.LT.(1.-D)) THEN
    GO TO 90
    ENDIF
C
    ESB=1.-AREA/S3/UF/(1.-D)
    IF(ESB.LT.0.0) THEN
    GO TO 115
    ENDIF
    IF(ABS(ESB-ESB0).LT.0.000000000000000000000001) THEN
    GO TO 110
    ENDIF
    ESB0=ESB
C
```



```

100  CONTINUE
      WASH=BI
      IF (ABS(WASH-SURV).LT.0.0001) THEN
          GO TO 130
      ENDIF
      BI=(WASH+SURV)/2.0
      GO TO 60
110  IF (WASH.GT.0.0) THEN
          GO TO 120
      ENDIF
115  SURV=BI
      BI=BI+Z
      IF (BI.GT.1.0) THEN
          GO TO 150
      ENDIF
      GO TO 60
120  SURV=BI
      IF (ABS(WASH-SURV).LT.0.0001) THEN
          GO TO 130
      ENDIF
      BI=(WASH+SURV)/2.0
      GO TO 60
130  WRITE(*,140)UF,BI,ESB
      WRITE(4,140)UF,BI,ESB
140  FORMAT(1X,3F9.5)
150  CONTINUE
      STOP
      END

```

C
C
C

```

SUBROUTINE RKG(H,T,U,X,S1,D,B,UF,XF,A,GAMA)
IMPLICIT REAL*8 (A-H,O-Z)
F(T,U,X)=A*(UF-U)/(S1*D+T)-X*U*B/
& (1.+U+GAMA*U*U)
G(T,U,X)=A*(XF-X)/(S1*D+T)+X*U*B/
& (1.+U+GAMA*U*U)
DF1=H*F(T,U,X)
DG1=H*G(T,U,X)
DF2=H*F(T+H/2.,U+DF1/2.,X+DG1/2.)
DG2=H*G(T+H/2.,U+DF1/2.,X+DG1/2.)
DF3=H*F(T+H/2.,U+DF2/2.,X+DG2/2.)
DG3=H*G(T+H/2.,U+DF2/2.,X+DG2/2.)
DF4=H*F(T+H,U+DF3,X+DG3)
DG4=H*G(T+H,U+DF3,X+DG3)
U=U+(DF1+2.*DF2+2.*DF3+DF4)/6.
X=X+(DG1+2.*DG2+2.*DG3+DG4)/6.
T=T+H

```

RETURN
END