Spring 6-30-1991

A comparative analysis of the efficacy of zero-order, first-order and Monod kinetic models in representing raw aerobic biodegradation data

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A Comparative Analysis of the Efficacy of Zero-Order, First-Order and Monod Kinetic Models in Representing Raw Aerobic Biodegradation Data

by

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NJIT Masters Thesis
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Date: June 17, 1991

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1. Abstract

A total of 148 raw aerobic biodegradation data sets from batch and continuous stirred-tank reactors were extracted from the open literature and previous NJIT MS theses. Kinetic analysis of each of these data sets was performed with respect to the following commonly-used empirical models: (1) zero-order, (2) first-order, and (3) Monod. Two constant-biomass versions of each model were evaluated; one in which So (i.e., the boundary condition for substrate concentration at time equal to zero) was assumed to be equal to the measured value of the initial substrate concentration and the other in which So was treated as a regressable parameter. Where adequate biomass concentration data were available, variable-biomass versions of each model, in which So was assumed to be equal to the initial substrate concentration, were also evaluated. Each data set was categorized within one of nine different biodegradation data types and discussed with respect to the advantages and disadvantages of each model evaluated for the given data type. Model selection recommendations were given for each data type.

A theoretical analysis of the effects of variations in raw biodegradation data on the corresponding regression results was performed for the constant- and variable-biomass models. The effects of random experimental error, number of data points, sampling regularity and substrate concentration range were evaluated. The impact of erroneous models on reactor sizing was also demonstrated.

2. Introduction

Chemical reactors assume many forms in a variety of industries. Regardless of the type of application, they are typically the focal point of a given process. Their proper design is of critical importance to the overall performance and economics of a process. This is just as true for wastewater treatment plants as it is for any conventional chemical or petrochemical process plant.

Of primary importance to the efficient design and operation of a chemical or biochemical reactor is a kinetic model which is consistent with physical reality. Biochemical reactions, which rely on the metabolic pathways of microorganisms, are inherently much more difficult to mechanistically model than conventional chemical reactions. No universal theoretical equation currently exists which can reasonably represent a cell's metabolic processes. As a result, academia and industry alike typically resort to empirical equations such as the zero-order, first-order, and Monod to model biochemical reactions. Their choice of which model to use in a given situation, however, has tended to be haphazard and lacking in scientific consistency.

The purpose of this thesis is to address this issue and to provide a foundation for the selection of empirical models for aerobic biodegradation reactions. A complementary objective of this thesis is to elucidate the relationship between the quantity/quality of experimental data and model selection, which, in turn, should provide further insight into the critical aspects of experimental data measurement.

3. Scope

This thesis is best viewed as being composed of two parts. The first part involves an extensive review of the literature for raw aerobic biodegradation data. The retrieved data are fit to constant-biomass versions of zero-order, first-order, and Monod kinetic models using linear regression analysis. Two variations of each model type are investigated. One in which regression is forced through the initial value of substrate concentration and the other in which initial substrate concentration is treated as an additional regressable parameter. Variable biomass versions of the zero-order, first-order, and Monod kinetic models are also evaluated using linear regression analysis for the cases in which adequate biomass concentration data are available.

The purpose of this first part of the thesis is two-fold: (1) to provide insight into the different aerobic biodegradation data types (i.e., substrate concentration vs. time curves) attained in industrial and academic research under a wide range of experimental conditions (e.g., substrate/biomass types and concentrations, temperature, and pH), and (2) to determine the advantages/disadvantages of each model for a given data type. Both batch reactor and continuous stirred-tank reactor aerobic biodegradation data are considered.

The second part of the thesis entails a theoretical analysis of the effects of variations in raw biodegradation data on the corresponding regression results for the constant- and variable-biomass models. The effects of experimental error, number of data points, sampling regularity and substrate concentration range are evaluated. This analysis will provide additional insight into the applicability of the above models in different situations, as well as give a better understanding of the critical aspects of experimental data measurement with respect to kinetic analysis.

4. Theory

In biological wastewater treatment, bacteria and other microorganisms break down and metabolize the soluble and colloidal organic material thereby reducing the BOD (biochemical oxygen demand) and COD (chemical oxygen demand) to acceptable levels. At the molecular level, this is an extremely complex process; substrate is absorbed by the bacterial cell along with other essential nutrients (e.g., N, P, oxygen, minerals, and cofactors), wherein it is acted upon by a myriad of enzymes as part of the cell's metabolism, ultimately yielding various amounts of cell growth and carbon dioxide or soluble nondegradable residue. Theoretical models are, as yet, unable to adequately represent the microscopic phenomena which occur. As a result, empirical equations are typically used to model the relationship between substrate concentration and time without regard for the actual mechanisms taking place.

The zero-order, first-order, and Monod equations are the most commonly used (i.e., by academia and industry) empirical models in the kinetic analysis of aerobic biodegradation data. Assuming that the organic substrate is the limiting reagent (i.e., all other nutrients are supplied in excess) and that no diffusion or mass-transfer limitations exist (i.e., the reaction is kinetically controlled), the order of the biodegradation reaction will depend on the concentration of substrate relative to that of the bacterial biocatalyst. At high

ratios of substrate to biocatalyst,the biodegradation rate will be limited by bacterial concentration and should be independent of substrate concentration (i.e., zero-order). At low ratios, substrate concentration is limiting relative to bacterial concentration and the biodegradation rate becomes proportional to substrate concentration (i.e., first-order). For ratios spanning both the zero-order and first-order regions, the shifting order kinetics of the Monod equation[1] will apply.

The mathematical derivation of the kinetic expressions used as a basis for the linear regression of biodegradation rate constants from batch reactor and continuous stirred-tank reactor data are presented in detail in Appendices A and B, respectively. Table 1 summarizes the integrated kinetic expressions used for batch reactor data analysis. The parameters in these equations (i.e., a, b, and c) are determined by linear regression using the method of least-squares analysis (refer to Appendix A, page A-17).

The above integral treatment of substrate concentration, S, versus time, t, batch reactor data is used in this thesis as opposed to the more empirical differential treatment for the following reasons: (1) the inherent difficulty in accurately determining the differential, dS/dt, either analytically (by first fitting the data with a polynomial function) or graphically, and (2) the inability of the differential approach to fit anything other than nth-order kinetics (i.e., analysis of Monod equations is not possible).

Table 1

Batch Reactor Kinetic Expressions

Model	Integrated Kinetic Expression*
Constant Biomass:	
Zero-order (1-parameter)	$t = (1/k)(So-S)$ $= (a)(x)$
Zero-order (2-parameter)	$t = (-1/k)S+(So/k)$ $= (a)x+(b)$
First-order (1-parameter)	$t = (1/k)(\ln(So/S))$ $= (a)(x)$
First-order (2-parameter)	$t = (-1/k)\ln S+((\ln So)/k)$ $= (a) x +(b)$
Monod (2-parameter)	$t = (K/k)\ln(So/S)+(1/k)(So-S)$ $= (a) x +(b) z$
Monod (3-parameter)	$t = (-K/k)\ln S+ (-1/k)S+((K/k)\ln So+(So/k))$ $= (a) x + (b)z+(c)$
Variable Biomass:	
Zero-order (1-parameter)	$t = (1/koYc)(\ln((Bo+YcSo-YcS)/Bo))$ $= (a)(x)$
First-order (1-parameter)	$t = (-1/(ko(Bo+YcSo)))(\ln(BoS/((Bo+YcSo-YcS)So)))$ $= (a)(x)$
Monod (2-parameter)	$t = (K/(ko(Bo+YcSo)))(\ln((Bo+YcSo-YcS)So/(BoS)))$ $= (a)(x)$ $+ (1/(koYc))(\ln((Bo+YcSo-YcS)/Bo))$ $+ (b)(z)$

* a, b, and c are regressable parameters; t, x, and z are given data(refer to Appendix A, page A-3, for clarification of nomenclature).

In the least-squares analyses performed in this thesis, minimization of model error is performed with respect to the independent variable, t, and not the dependent variable, S. This is done because all of the models being considered are not linear and explicit with respect to S, whereas they are with respect to t. The statistic $\Sigma(t-tcalc)^2$ will, therefore, provide a common basis of comparison between models.

The kinetic expression that minimizes the sum of the squares of the discrepancies between model predictions and measured values is the one with the highest probability of being correct. The statistic $\Sigma(t-tcalc)^2$ alone does not, however, indicate whether a given model is a good fit; it only tells which of the models considered is statistically best. A model can be considered a good fit to a set of data if the experimental points are normally distributed around the predicted curve due to random error during measurement. This can be readily detected graphically in a plot of substrate concentration, S, versus time showing both experimental data and the predicted curves. The calculation of S as a function of time is straightforward (once the parameters have been regressed) for the zero- and first-order models since these expressions are explicit with respect to S. The Monod models, however, are not explicit in S and therefore require trial-and-error solution of the variable. The Newton-Raphson method is used here for this purpose (refer to Appendix A, page A-23).

It should be noted that slightly different results would be obtained if the regression analyses were performed relative to the dependent variable, S, rather than the independent variable, t. In a plot of S versus t, regression with respect to t will minimize the error in the horizontal direction between the given model and data, whereas regression with respect to S would minimize the error in the vertical direction. While the standard convention is to perform regression with respect to the dependent variable and plot it on the ordinate versus the independent variable, it was not followed here. Regression with respect to t in this thesis facilitates a straightforward statistical comparison between the models being investigated. The graphical results, however, are presented in the standard manner of S versus t for ease of interpretation. This fact should be remembered when reviewing results since the errors between the predicted curves and experimental data will be minimized in the horizontal direction with respect to t, as opposed to the more common approach of error minimization in the vertical direction relative to the dependent variable, S.

Table 2 summarizes the kinetic expressions used for continuous stirred-tank reactor analysis. The regression of kinetic parameters and subsequent analysis of results are performed in the same manner as the batch reactor data analysis. The calculation of S as a function of time for the Monod models, however, is slightly simpler, requiring solution by quadratic formula only.

Sample calculations for the regression of kinetic parameters from batch reactor data are shown for both the constant- and variable-biomass models in Appendix C. Also included are printouts of LOTUS 123 spreadsheets which were developed to facilitate these tedious calculations (refer to page C-16). Calculations for the regression of kinetic parameters from continuous stirred-tank reactor data are methodically analogous to that shown for the batch reactor and, hence, sample calculations for them are not included.

It should be noted that the higher-parameter versions of the variable-biomass models (i.e., where So is treated as a regressable parameter) were not considered as part of the base group of models studied in this thesis. Analysis of these models requires non-linear regression techniques which are outside the main scope of this work.

Table 2

CSTR Kinetic Expressions

Model	Kinetic Expression*
Constant Biomass:	
Zero-order (1-parameter)	(V/Q) = (1/k)(Si-Se) = (a)(x)
Zero-order (2-parameter)	(V/Q) = (-1/k)Se+(Si/k) = (a)x +(b)
First-order (1-parameter)	(V/Q) = (1/k)((Si-Se)/Se) = (a)(x)
First-order (2-parameter)	(V/Q) = (Si/k)(1/Se)+(-1/k) = (a)(x)+(b)
Monod (2-parameter)	(V/Q) = (K/k)((Si-Se)/Se)+(1/k)(Si-Se) = (a)(x)+(b)(z)
Monod (3-parameter)	(V/Q) = (SiK/k)(1/Se)+(-1/k)Se+((Si-K)/k) = (a)(x)+(b)z +(c)
Variable Biomass:	
Zero-order (1-parameter)	(V/Q) = (1/ko)((Si-Se)/ (Bi+Yc(Si-Se))) = (a)(x)
First-order (1-parameter)	(V/Q) = (1/ko)((Si-Se)/((Bi+Yc(Si-Se))Se)) = (a)(x)
Monod (2-parameter)	(V/Q) = (K/ko)((Si-Se)/((Bi+Yc(Si-Se))Se)) = (a)(x) +(1/ko)((Si-Se)/(Bi+Yc(Si-Se))) +(b)(z)

* a, b, and c are regressable parameters; (V/Q), x, and z are given data (refer to Appendix B, page B-3, for clarification of nomenclature).

5. Literature Search

An extensive search of the scientific literature was conducted for raw aerobic biodegradation data resulting in the extraction of 63 sets of data from 24 articles encompassing 8 different trade journals. Batch and CSTR data from both mixed-culture and single-culture systems were considered, providing each set consisted of a minimum of 4 points. A listing of the literature references used is given in Appendix D (page D-3), while a breakdown by data type is provided in the following table:

	Number of Data Sets*	
System	Batch Reactor Data	CSTR Data
Mixed Culture	39(7)	4(4)
Single Culture	16(6)	4(4)

*Values in parentheses refer to the number of data sets for which variable-biomass concentration data were available.

In addition to the above literature data, 85 sets of raw aerobic biodegradation data were extracted from a total of six previous New Jersey Institute of Technology MS Theses (refer to Appendix E, page E-3, for a listing). All of the data sets were for batch-reactor activated-sludge systems, while 18 of the total included variable-biomass concentration data.

All in all, a broad base of data involving 27 different substrates was compiled for this study.

The treatment of the above-mentioned data with respect to kinetic analysis and modelling by the respective authors varied dramatically. Of the 24 articles used, 9 performed no kinetic analysis at all (references 7, 9, 14, 16, 17, 21-24 in Appendix D, pages D-3 through D-5). These papers were concerned more with the feasibility of biodegradation of specific substrates and the underlying biological mechanisms and metabolic pathways than with modelling of the data. The remaining 15 papers, on the other hand, used a myriad of different equations to model their biodegradation data: zero-order (references 1,4), first-order (references 3, 10, 12, 13, 18), second-order (reference 6), Monod (references 3, 15, 19), modified versions of Monod to account for substrate inhibition (references 2, 8, 11, 15), and more sophisticated mechanistic models (references 5, 15, 20). A lack of consistency in the selection and application of models is readily apparent.

6. Discussion of Regression Analysis Results

The raw aerobic biodegradation data extracted from the literature sources and previous New Jersey Institute of Technology MS Theses were regressed using the method of least-squares analysis for the constant- and variable-biomass versions (the latter, where applicable) of the zero-order, first-order, and Monod kinetic models with the results from the data sources being compiled in Appendices D and E, respectively. Both appendices include lists of the relevant references and indices of the results contained therein. The results are presented within the appendices in the form of summary sheets for each raw biodegradation data set studied. Each summary sheet presents the raw data used, the literature reference from which it was extracted, the conditions under which the data were experimentally determined, and the corresponding regression analysis results (i.e., regressed kinetic rate constants and sum-of-the-squares of the errors for each model).

The discussion of the regression analysis results is performed in subsections according to reactor (i.e., batch and CSTR) and culture (i.e., mixed and single species) types. To make the discussion of these results more tractable, the data sets are grouped and discussed according to major trends in biodegradation data type (e.g., zero-order, first-order, Monod, etc.). Anomalies are also noted, along with the capabilities/inabilities of each of the models studied to represent the data. Where applicable, appropriate comparisons and comments are made with respect to kinetic analyses performed in the literature references utilized in this thesis.

6.1 Batch Reactor Data--Mixed Culture Systems

The bulk of the raw biodegradation data available in the literature is derived from batch reactors because they are much simpler than continuous reactor systems to set up, run and obtain kinetic data. Furthermore, ideal batch reactor behavior in terms of perfectly-mixed conditions can be, and for the most part is, closely approximated, thereby facilitating a relatively straightforward and reliable kinetic analysis. Of the 148 data sets studied in this thesis, 140 are for batch reactor systems.

Discussion of batch reactor biodegradation data within this thesis is subdivided according to the general categories of mixed- and single-culture systems to provide some insight into any differences which may be evident between the two cases with respect to kinetic modelling. Most of the batch reactor data sets studied here (i.e., 124 out of 140) utilized mixed cultures. The high percentage of biodegradation studies performed in the literature utilizing mixed cultures directly follows from the fact that virtually all wastewater treatment facilities and the environment, in general, operate under such conditions.

The raw biodegradation data types discussed in the following subsections are for the most part some variation of one of the two curves shown in Figure 1 providing that the substrate is limiting and that the reaction is kinetically controlled (i.e., diffusion and mass-transfer resistances are negligible). Curve 1 is for the case of constant biomass while Curve 2 is for the variable-biomass case with

Figure 1

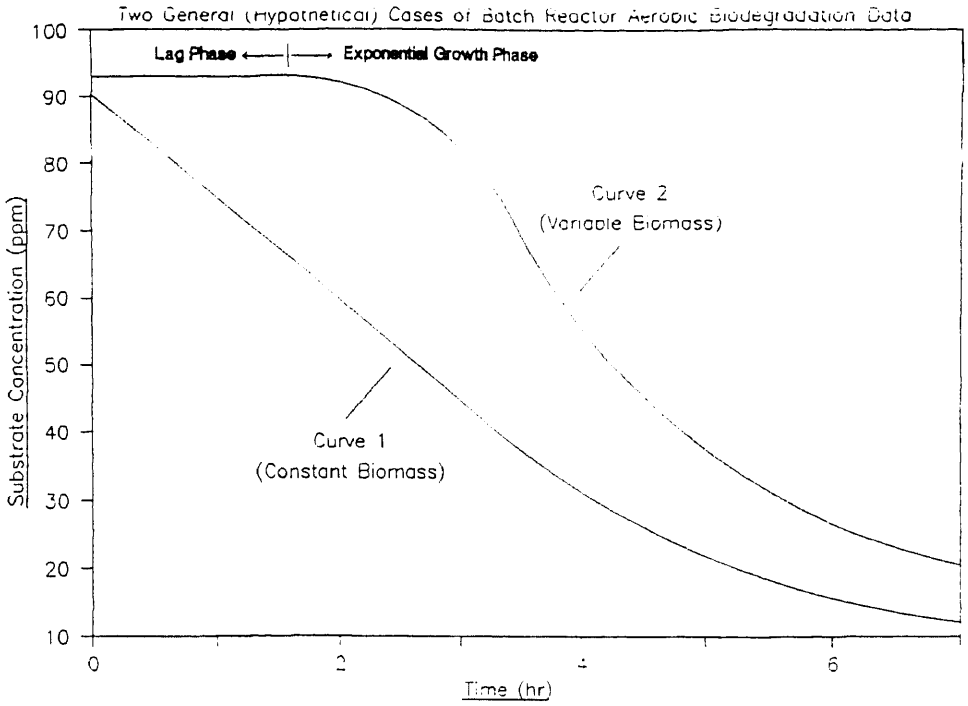
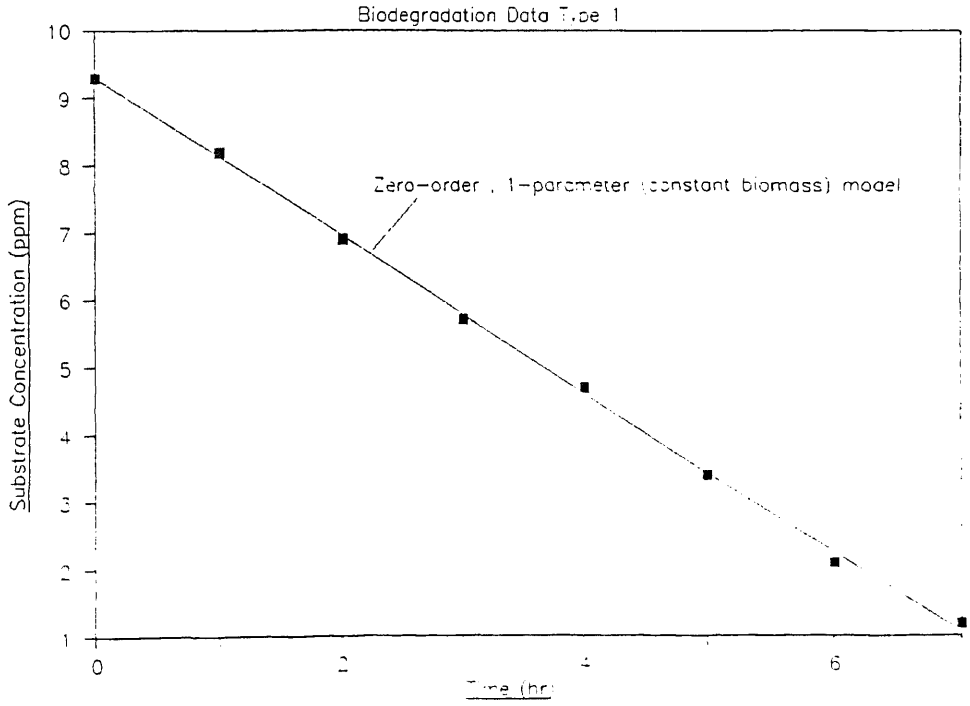


Figure 2



Source : Naik Thesis (data set #8B) ; refer to page E-50

both the lag phase and exponential growth phase for a typical bacterial culture being schematically presented. Depending on the portion of either curve over which a given data set is measured, it can be interpreted as being either the constant- or variable-biomass form of the zero-order, first-order or Monod kinetic models. The designation of a given data set as a specific biodegradation data type is not always definitive because of a combination of factors such as experimental error, missing data points, and measurement over ranges intermediate between two different data types.

6.1.1 Data Type 1 (Zero-Order, Constant Biomass)

The first biodegradation data type to be discussed is the zero-order, constant-biomass type presented in Figure 2. The data set shows substrate concentration, S, to be a linear function of time, t, with very little data scatter and is well represented by the zero-order, 1-parameter, constant-biomass model. This data type can be expected when S is high relative to the viable biomass concentration. At first glance, the data in Figure 2 might not be expected to follow zero-order kinetics because of the low S range (i.e., 1.2-9.3 ppm) covered for an activated sludge system where the total biomass concentration, B, is high (e.g., typically 2000-5000 ppm). The activated sludge, however, was not acclimated to the substrate and, as such, only a very small proportion of the bacterial population was capable of metabolizing the substrate. It is readily apparent that the prediction of data type cannot be generalized from the values of

S and B alone; knowledge of the population of viable bacteria is also required.

A comparison of the constant-biomass versions of the zero-order, first-order, and Monod kinetic models in representing the data from Figure 2 is presented on page E-80 in terms of the statistics $\Sigma(t\text{-}tcalc)^2$ and $\Sigma(S\text{-}Scalc)^2$ (note--the values listed on the summary sheets in Appendices D and E are normalized with the sum-of-the-squares of the error of the relevant parameter being divided by the number of data points used). The former statistic is more pertinent in this study than the latter since the least-squares analyses were all performed with respect to the explicit variable t, and not S. The latter statistic is provided for comparison purposes only. In terms of the data shown in Figure 2, the best models based on the statistic $\Sigma(t\text{-}tcalc)^2$ are, in order: (1) Monod (3-parameter) or M3, (2) Monod (2-parameter) or M2, (3) zero-order (2-parameter) or Z2, (4) zero-order (1-parameter) or Z1, (5) first-order (2-parameter) or F2, and (6) first-order (1-parameter) or F1. **The difference between the first four models is minimal with the regressed curves all being virtually identical to that shown in Figure 2.** The first-order models, F1 and F2, are statistically and visually much worse (refer to Figure 3).

The Monod model ($-dS/dt = kS/(K+S)$) reduces to zero-order kinetics when $S \gg K$, as is the case in Figure 2 with the value of k being virtually the same for both model types. From a regression

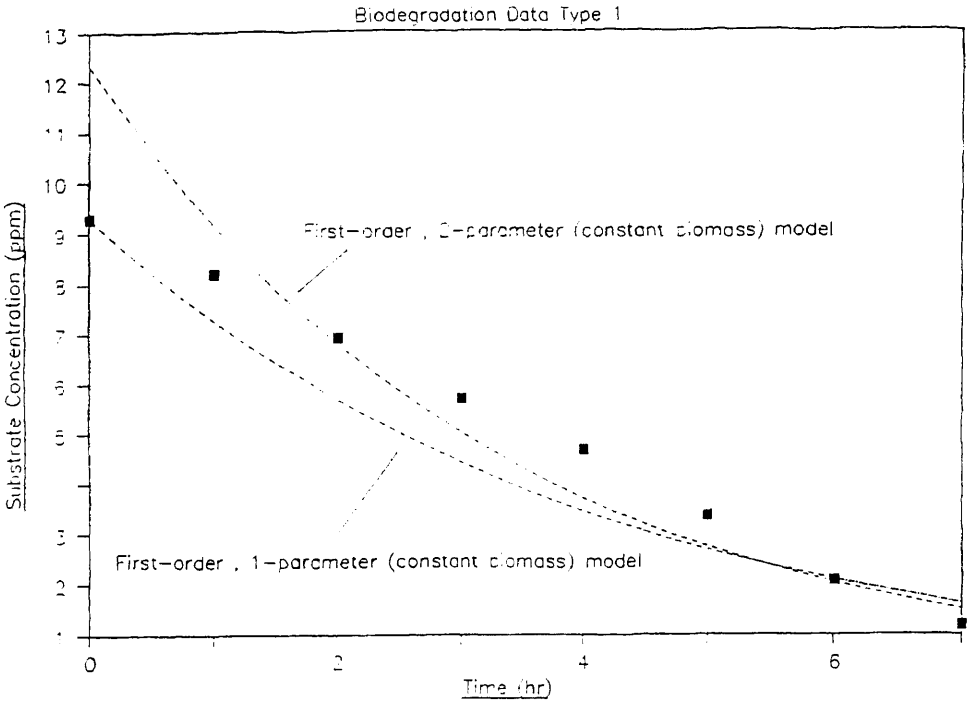
analysis perspective, the Monod model is expected to be statistically better than the zero-order model in representing raw aerobic biodegradation data because of the regressable parameter K which gives the Monod model an additional degree of freedom in fitting the data. For truly zero-order kinetics with ideal data (i.e., no systematic or random errors of measurement), the two models would yield identical results. But since some degree of experimental error is always present, the Monod model will always be statistically better than the corresponding zero-order model (i.e., M3 vs. Z2 and M2 vs. Z1). In general, the more scatter in the data, the greater the difference expected. In the case of Figure 2, the difference between Monod and zero-order models is small because of the apparent high accuracy of the raw data.

In line with the discussion of the above paragraph, the models which regress for So will yield statistically better results than those which assume So = S(t=0) because of the extra degree of freedom provided by the additional regressable parameter in the fitting of a model to a given set of data. For ideal data of a given kinetic type (i.e., zero-order, first-order or Monod), the two cases would yield identical results. But for real data with experimental uncertainties, the higher-parameter versions are better with the differences becoming more pronounced as experimental error increases. In the case of Figure 2, the higher-parameter versions of the Monod and zero-order models are only marginally better because of the apparent minimal experimental error present.

The regressed first-order models for the data shown in Figure 2 are presented in Figure 3. It is apparent that both versions are incorrect representations of reality. The 1-parameter version, F1, fits the initial point So = S(t=0) and approximates the latter points while underpredicting the rest. The curvature is inherent in the model (S = So*exp(-kt)) and the preferential fit of the latter region over the intermediate is attributed to the logarithmic function (i.e., x = ln(So/S)) used in the regression analysis which naturally favors the latter (lower S value) points (refer to page C-6). The 2-parameter version, F2, also fits the latter points in the same manner and for the same reason, but averages the error over the rest of the data range to minimize $\Sigma(t-tcalc)^2$ by excessively over-predicting So. F2 is statistically better in terms of $\Sigma(t-tcalc)^2$, as expected, but worse in terms of $\Sigma(S-Scalc)^2$. Slightly different results would be obtained if the least-squares analyses were performed to minimize the error in S; F2 would be visually better with a lower value of $\Sigma(S-Scalc)^2$, but worse in terms of $\Sigma(t-tcalc)^2$. In any case, no first-order model could well represent the zero-order kinetics observed in Figure 2.

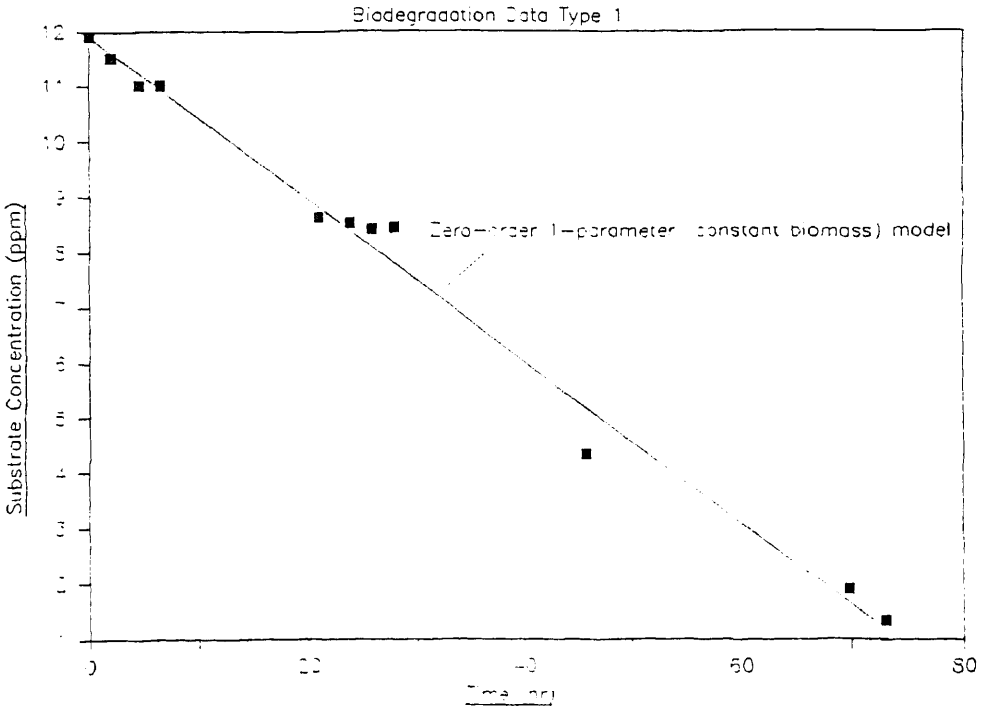
Another example of biodegradation data type 1 is presented in Figure 4. It is analogous to the data set in Figure 2 in that no first-order effect is apparent even though the S range is low (i.e., 1.3-11.9 ppm) relative to B (i.e., 3800-4100 ppm). This is

Figure 3



Source : Naik Thesis (data set #8B) ; refer to page E-80

Figure 4



Source : Gonnebathula Thesis (data set #3B) ; refer to page E-25

attributed to the fact that only a very small percentage of the total biomass measured is viable for the substrate in question, 2,6-dichlorophenol, which is reputed to be relatively resistant to bacterial utilization.

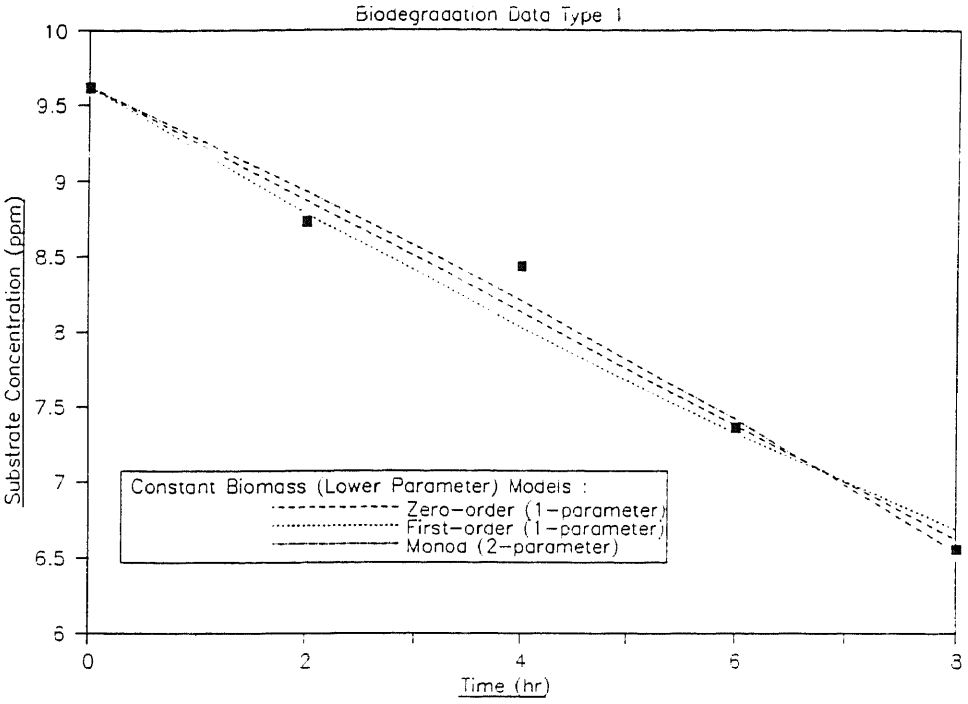
The data set in Figure 4 has an increased amount of scatter compared to that in Figure 2. This increase in data scatter results in a dramatic increase in the average sum-of-the-squares of the error in t for both the Monod and zero-order models, while having a significantly smaller effect on the first-order models. Although $\Sigma(t\text{-}tcalc)^2$ is still much higher for the first-order models than for either the zero-order or Monod, it is obvious that model differentiation and, hence, proper model selection becomes more difficult as uncertainties in experimental measurement increase.

Although the data set in Figure 4 shows significantly more scatter than the data set in Figure 2, the regressed curves for Z1, Z2, M2 and M3 all coincide with one another. This is the result of the experimental error in the data being approximately normally distributed around the predicted zero-order curve. The first-order curves are, in effect, identical to those shown in Figure 3 and are therefore not presented nor discussed further here.

Figures 5 and 6 graphically present the results from page E-97 for the lower- and higher-parameter constant-biomass models, respectively. This data appears to be the same type as the previous two sets discussed so far except with a much higher degree of scatter relative to the small S range covered. As mentioned previously, increased scatter makes model differentiation and proper model selection more difficult. Statistically, the sequence of models from best to worst is unchanged from the previous sets. The difference between best and worst (i.e, M3 and F1), however, is much less with Figures 5 and 6 showing all six curves to be reasonable over the S range covered. Extrapolation of any of the models considered outside of the measured range, however, would be extremely risky and ill-advised because of the low level of certainty on which model, if any, is correct; for lower values of S, the errors caused by selection of an incorrect model would be greatly magnified.

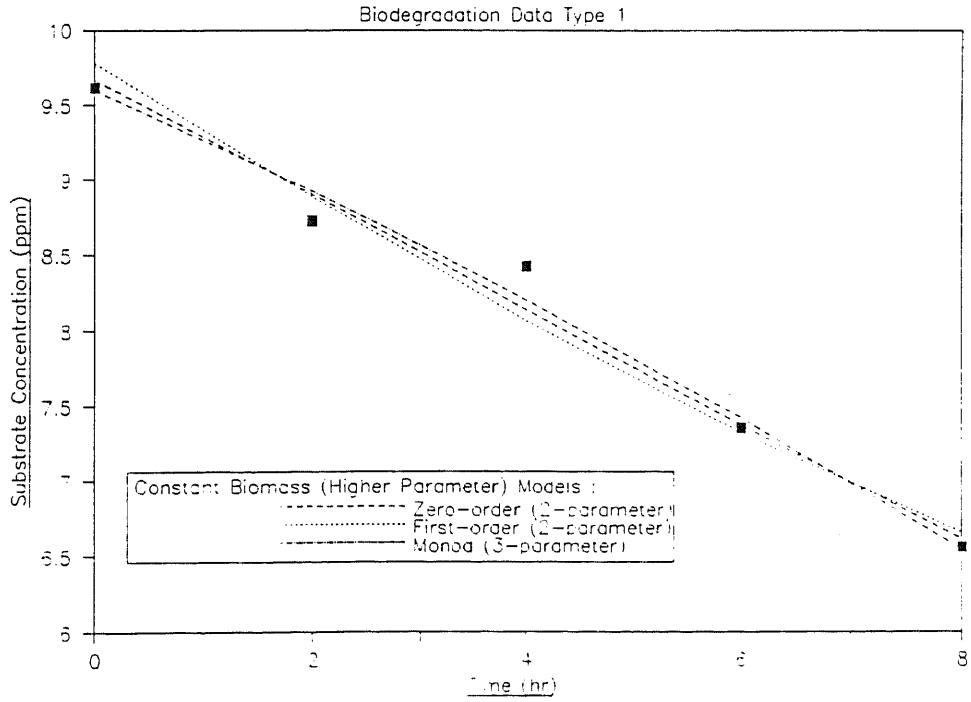
While the Monod models are statistically best (in all cases), the regression results on page E-97 indicate negative values of the kinetic parameter K for both the 2- and 3-parameter versions. A negative value of the rate constant K is physically uninterpretable and nullifies any theoretical basis in the Monod model derived from the Michaelis-Menten relationship[1]. Regression yields a negative value of K because the scatter in the data gives the effect of a slight downward slope. The Monod models minimize $\Sigma(t\text{-}tcalc)^2$ by using a

Figure 5



Source : Pak Thesis (data set #4) ; refer to page E-97

Figure 6

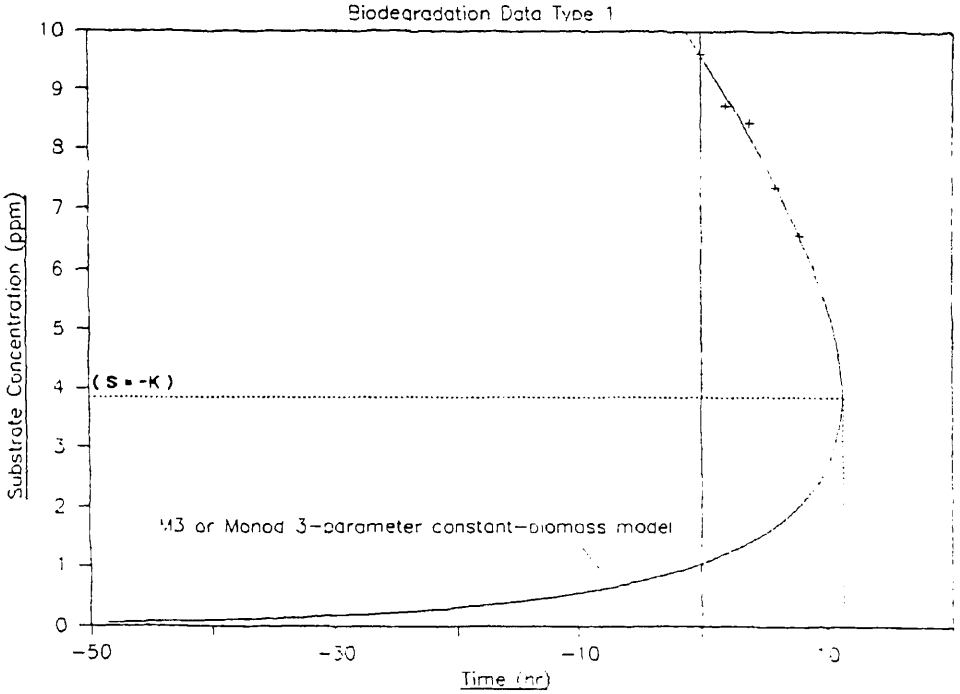


Source : Pak Thesis (data set #4) ; refer to page E-97

negative K to fit the apparent curvature rather than yielding the conventional first-order curvature obtained with a positive value of K. While the Monod models in Figures 5 and 6 fit the data over which they were regressed, extrapolation down to S values approaching the absolute value of K is not feasible as -dS/dt goes to infinity (i.e., -dS/dt indeterminate at S = -K), thereby limiting the practical usefulness of an already theoretically invalid model. This problem is displayed graphically in Figure 7 which shows an expanded version of the predicted M3 curve from Figure 6. The curve doubles back on itself at a value of S equal to the absolute value of K.

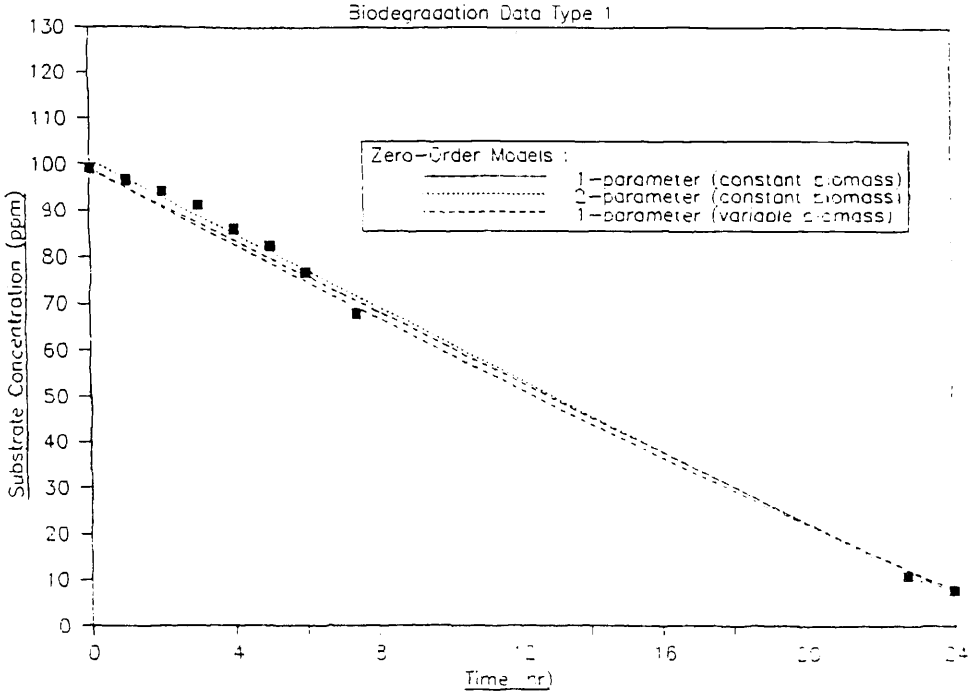
The Monod models have an approximately equal likelihood of regressing negative values for K as they do positive values for any zero-order kinetic data. The value of K for the case of zero-order kinetics is dependent solely on the scatter in the data resulting from experimental errors in their measurement and whether the overall set, as a result, is interpreted as having either a slight upward or downward curvature. Because of this problem with the Monod models in representing zero-order kinetics, the zero-order models are, in general, best for interpolating type 1 data even though the Monod are statistically always somewhat better. Extrapolation of the zero-order models below the range in which the kinetic parameters

Figure 7



Source : Pak Thesis (data set #4) ; refer to page E-97

Figure 8

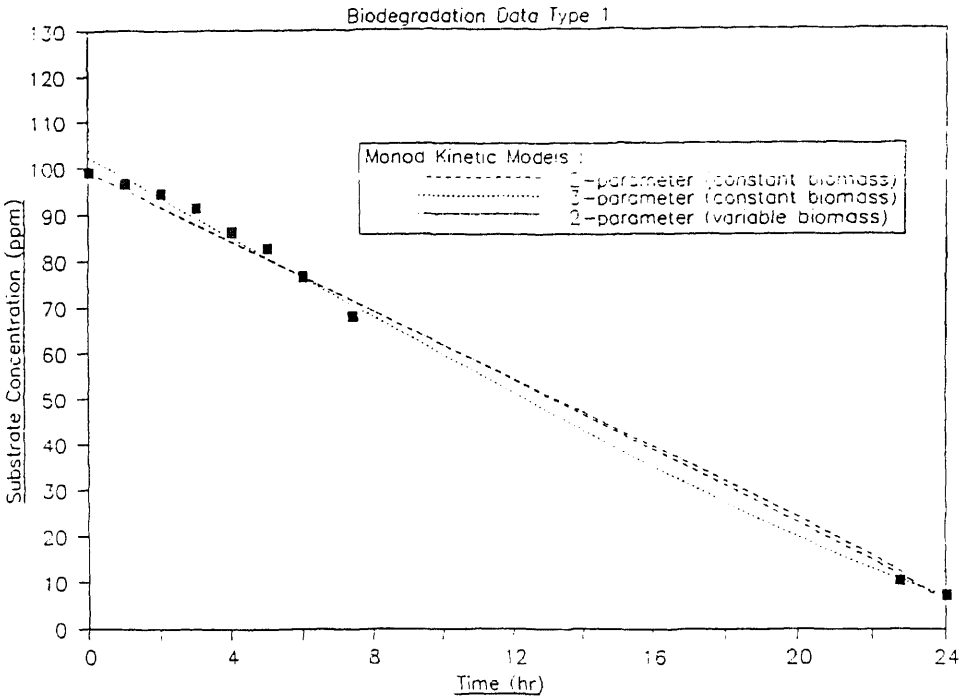


Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105

were regressed, however, is unrealistic since it predicts negative values of S for t>So/k. In reality, as S becomes smaller, it will asymptotically approach the t axis in an infinitely long "tail". Since most pollution problems require removals down to very low levels, final effluent concentrations are generally in the "tail". In such cases, a zero-order model can grossly underpredict the size of the reactor.

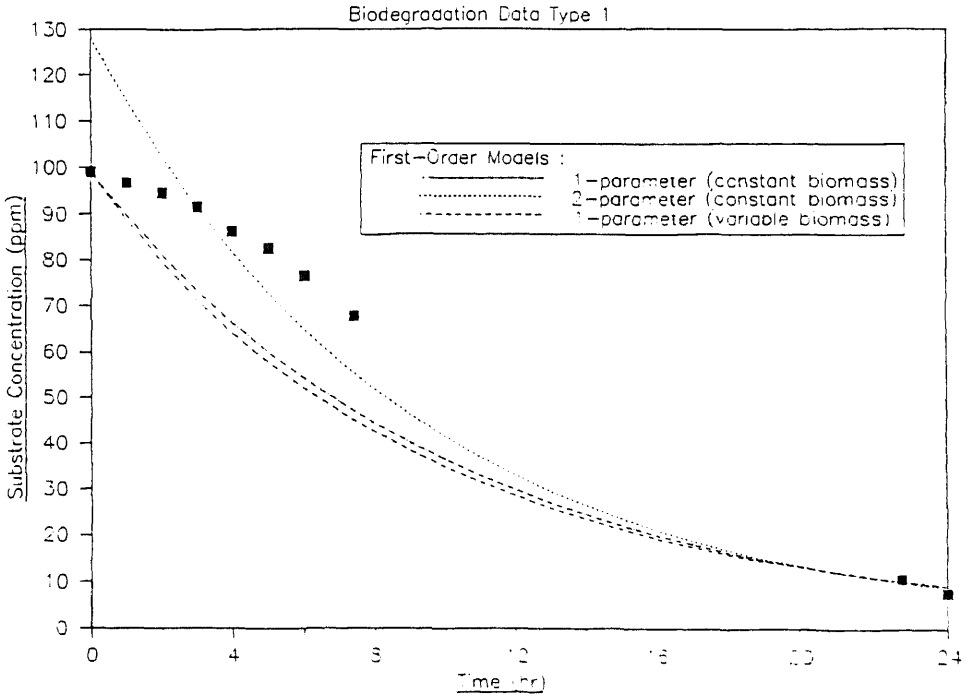
Figures 8-10 graphically represent the regression results summarized on pages E-104 and E-105. Unlike the cases discussed thus far, this system included biomass concentration data which facilitated regression analysis of the variable-biomass kinetic models. The variable-biomass models used in this thesis assume a linear relationship between biomass generated and substrate consumed, with the proportionality constant being designated as the yield coefficient (i.e., Yc = (B-Bo)/(So-S)). A value between 0 and 1 is typically expected. For this case, however, a negative value of Yc was calculated based on raw biomass data with a linear correlation coefficient of 0.86. The reason for the negative value of Yc is less likely inaccuracy in the measurement of B (because of a relatively high correlation coefficient) than the nature of the mixed-culture system itself. If the proportion of bacteria in a mixed-culture system capable of metabolizing a specific substrate is small (as is apparently so in this case), the "total" biomass concentration may decrease due to endogenous respiration while the level of substrate-specific bacterial concentration actually increases. The values of

Figure 9



Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105

Figure 10



Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105

Bo and Yc used in the variable-biomass models should be based on measurements of viable, and not total, biomass measurements in order to yield reliable regression results. Unfortunately, such measurements are not easily made for mixed-culture systems. The bulk of the variable biomass data utilized in this thesis is based on the dried weights of insoluble biomass. This method does not differentiate between living and dead cells, let alone viable ones. Pike and Carrington[2] showed that the percentage of total bacteria which are viable in various stages of wastewater treatment operations is typically on the order of only 1 to 3%. Furthermore, "weight" is not as reliable a measure of total biodegradation activity as "number of cells" because of the tendency of cells to fluctuate in size (via the creation/utilization of storage products) with slight changes in the environmental condition of the culture. Regardless of the aforementioned limitations and problems, analysis of the performance of the variable-biomass models in this thesis should provide considerable insight into their sensitivity to Bo and Yc, as well as their applicability and flexibility in different situations.

The best models for the data on pages E-104 and E-105 based on the statistic $\Sigma(t\text{-}tcalc)^2$ are in order: (1) M3, (2) Z2, (3) M2, (4) Z1, (5) Monod (variable biomass, 2-parameter) or MV, (6) zero-order (variable biomass, 1-parameter) or ZV, (7) F2, (8) F1, and (9) first-order (variable biomass, 1-parameter) or FV. Figures 8, 9 and 10 graphically present the results for the zero-order, Monod and

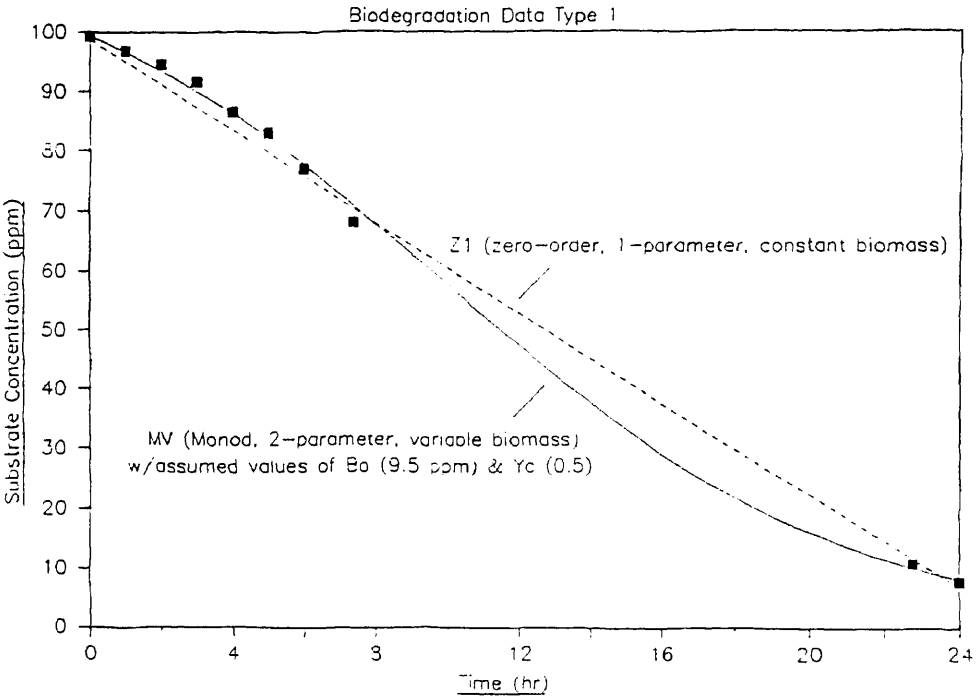
first-order models, respectively. Figures 8 and 9 show all the zero-order and Monod models to be reasonable given the quality/quantity of the data, while Figure 10 shows all the first-order models to be poor. As expected, the models with So as a regressable parameter are better than the corresponding constant-biomass models with So = S(t=0). In this case, the higher-parameter zero-order model, Z2, is even statistically better than the lower-parameter Monod, M2. Unexpectedly, the variable-biomass models are all statistically worse than the corresponding constant-biomass versions. With accurate values of Bo and Yc, the variable-biomass models should always be better than or equal to the corresponding lower-parameter constant-biomass versions as a result of the additional parameters representing catalyst concentration. The aforementioned problem with measurement of "total" and not "viable" biomass is the cause of the determination of an erroneous negative value for Yc which, in turn, accounts for the reduced performance of the variable-biomass models. Another problem with the measurement of "total" biomass (instead of "viable" biomass) in terms of the variable-biomass models is that the values of B are often so large that effectively constant-biomass behavior is predicted even when the S vs. t data indicate exponential growth. In the case of Figures 8-10, the variable-biomass models, although statistically worse than the corresponding lower-parameter constant-biomass versions (i.e., MV vs. M2, ZV vs. Z1 and FV vs. F1), are only slightly worse because B

decreases by only 15% over the S range covered thereby closely approximating constant-biomass behavior. Since the variable-biomass curves in Figures 8-10 are so similar to the corresponding constant-biomass curves, detailed discussion of the characteristics of the variable-biomass models and the effect of Bo and Yc upon them is reserved for subsequent examples where the phenomenon of exponential bacterial growth is visually more readily apparent.

Figure 9 shows all 3 versions of the Monod model to be reasonable for the data given. Both M2 and MV, however, yield negative values for K while M3 regresses a positive K. The 2-parameter models yield a negative K because of a slight downward bend in the data when forcing the curves through So = S(t=0). When the So restriction is relaxed in the case of M3, the data is interpreted as having a slight upward bend thereby accounting for the positive value of K being regressed.

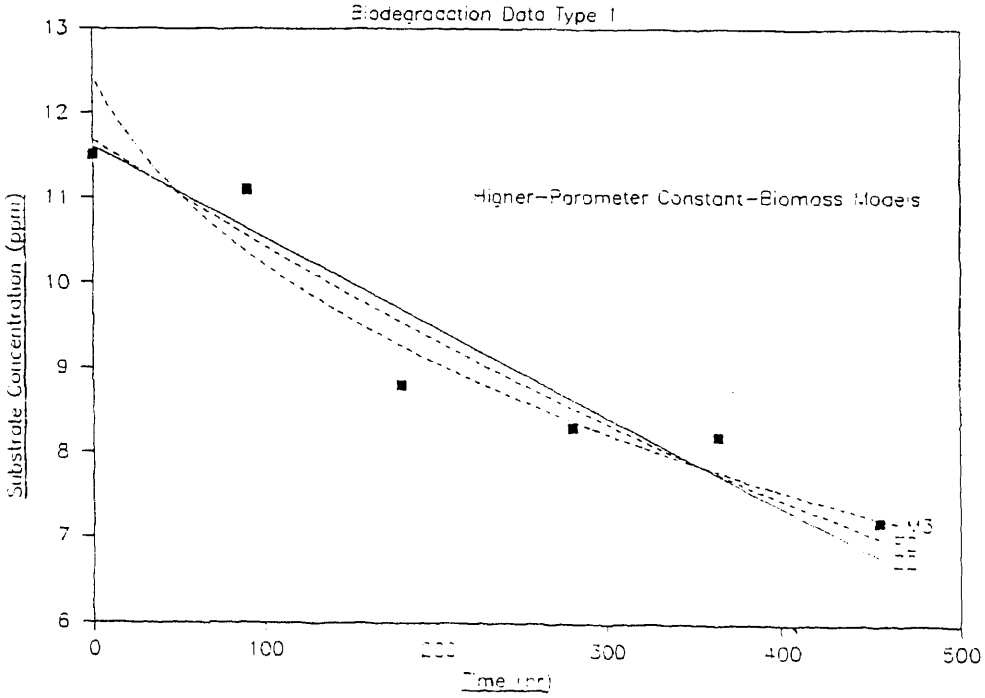
While the data in Figures 8-10 have been interpreted as type 1 (i.e., zero-order, constant biomass), significant uncertainty exists as to whether it is an accurate interpretation because of the missing gap of data between 8 and 24 hours. Figure 11 shows the data and Z1 curve along with a hypothetical MV curve for which values of Bo and Yc were arbitrarily selected so as to provide a good fit of the apparent subtle curvature in the data. The MV curve provides a visually and statistically better fit, and indicates that depiction of this

Figure 11



Source : Pak Thesis (data set #9) ; refer to pages E-104 & 105

Figure 12



Source : Salerno Thesis (data set #1), refer to pages E-107 & 108

data set as zero order may likely be incorrect. This case illustrates the necessity of measuring data at frequent intervals over the entire range of interest, when reliable kinetic modelling is desired, in order to reduce the probability of missing critical features of the S vs. t curve. Unfortunately, irregularity in data measurement was a common occurrence for the data extracted from the previous NJIT theses, specifically for systems which ran overnight. As a side note, a comparison of the two MV curves in Figures 9 and 11 demonstrate the importance of Bo and Yc accuracy on the performance of the variable-biomass model.

Figure 12 graphically presents the higher-parameter constant-biomass models for the data set shown on page E-107 (the corresponding variable-biomass results are shown on page E-108). This set has a very high degree of data scatter and covers a small S range thereby making model differentiation impossible (compare $\Sigma(t\text{-}tcalc)^2$ and $\Sigma(S\text{-}Scalc)^2$ on pages E-107 and E-108). While this data set is arbitrarily designated as type 1, the Monod models predict curvature in excess of first order for each case (M2 being the only one shown in Figure 12). As a result of the interpretation of the data set by the Monod models as greater than first-order, M2, M3 and MV all regress negative values for the kinetic parameters k and K. This phenomenon is discussed in greater detail in later sections where its occurrence is more commonplace.

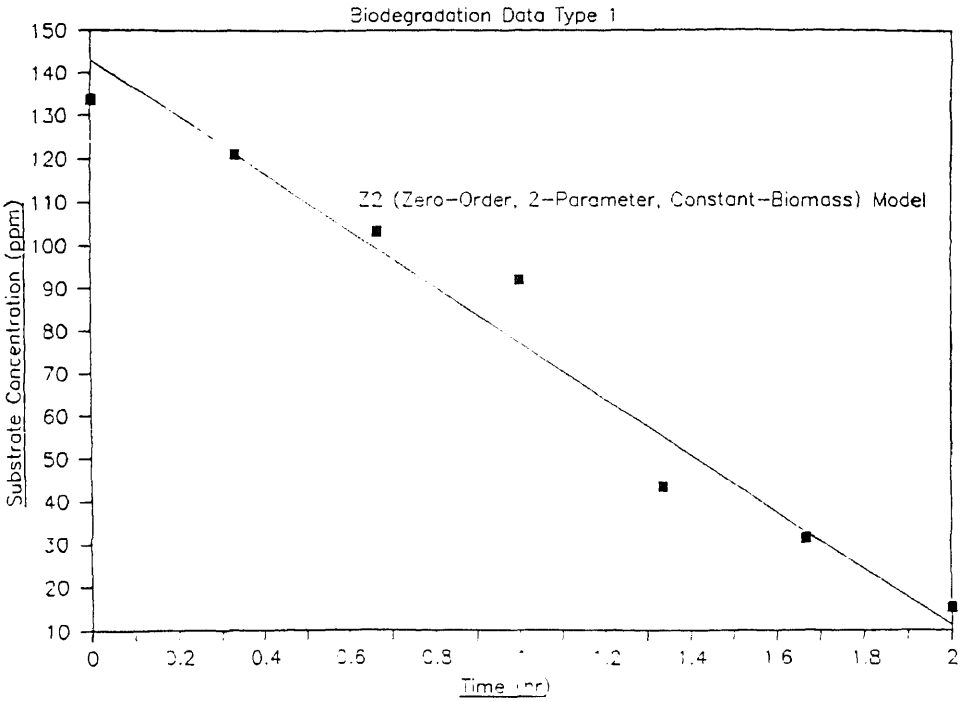
In addition to the 5 data sets discussed thus far, 4 more of the data sets reviewed were interpreted as type 1. Each set of raw data along with the corresponding regressed Z2 curves is presented in Figures 13 and 14. None of these data sets are of good quality. All 4 have a high degree of data scatter while the latter 3 (i.e., those in Figure 14) suffer from missing gaps of data over the range of S studied. The Monod models regress negative values of K for all 4 cases.

6.1.2 Data Type 2 (First-Order, Constant Biomass)

The second aerobic biodegradation data type to be discussed is the first-order, constant-biomass type shown in Figure 15 to be well represented by the F2 curve. Theoretically, first-order kinetics are expected for systems such as this one where the substrate concentration is low (i.e., <10 ppm) relative to biomass concentration (i.e., activated sludge), assuming all other nutrients are supplied in excess and that no mass-transfer limitations exist.

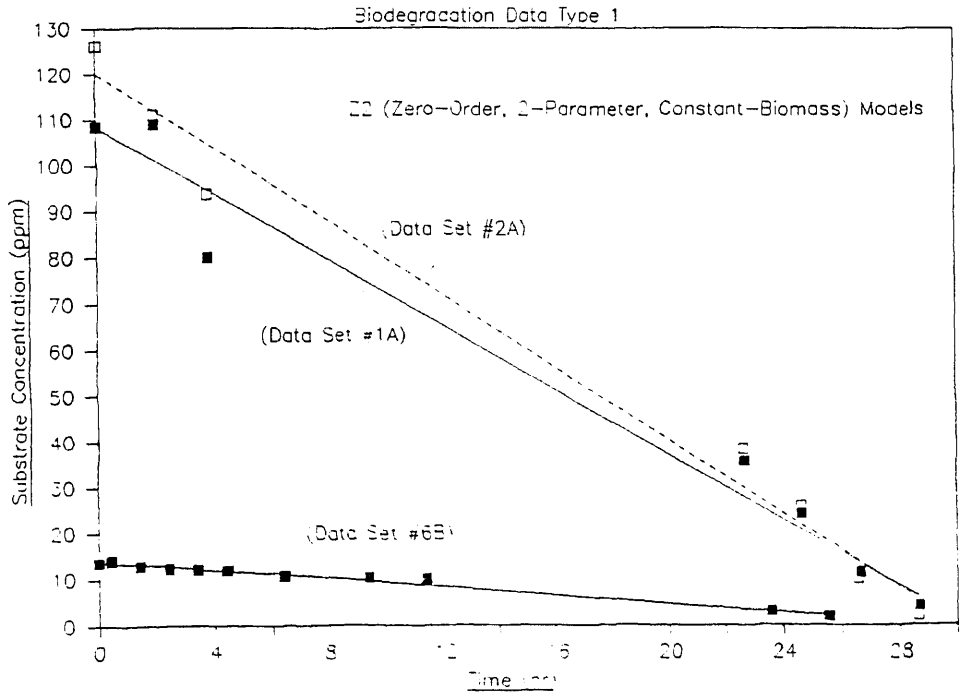
A comparison of the constant-biomass versions of the zero-order, first-order and Monod kinetic models in representing the data shown in Figure 15 is tabulated on page E-65. Statistically, the best models based on minimization of $\Sigma(t\text{-}tcalc)^2$ are in order: (1) M3, (2) M2, (3) F2, (4) F1, (5) Z2, and (6) Z1. The regressed results for the lower-parameter models are presented graphically in Figure 16. The corresponding higher-parameter models are virtually identical to those shown in Figure 16 (due to minimal data scatter) and are therefore not shown.

Figure 13



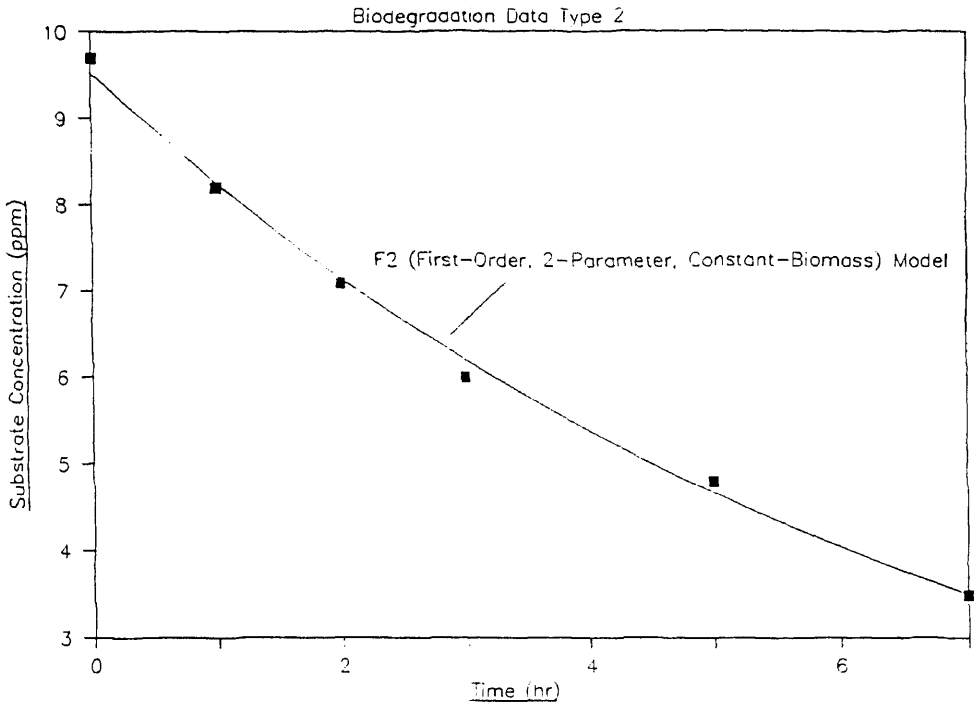
Source : Colish Thesis (data set #1) ; refer to pages E-6 & 7

Figure 14



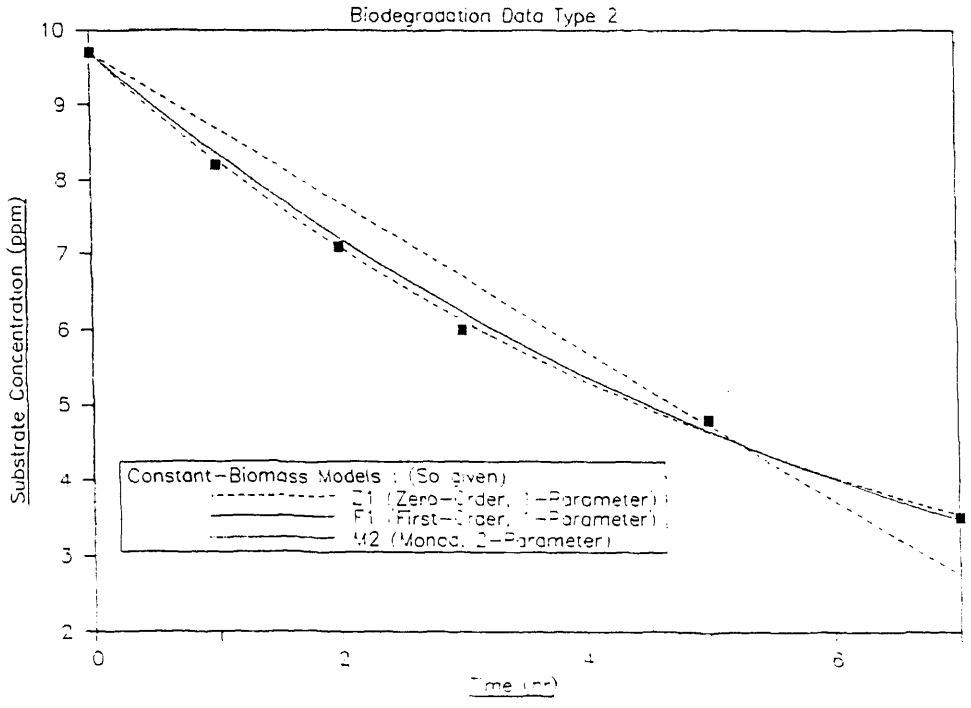
Source : Gonnabathula Thesis ; refer to data sets #1A, #2A & #6B on pages E-20, 22 & 31, respectively.

Figure 15



Source : Naik Thesis (data set #3B) ; refer to page E-65

Figure 16



Source : Naik Thesis (data set #3B) ; refer to page E-65

The Monod models, as before for zero-order data (i.e., data type 1), yield the statistically best results for first-order data. Whereas the Monod model (i.e., $-dS/dt = kS/(K+S)$) reduces to zero-order kinetics for high substrate concentrations (i.e., $S>>K$), it assumes first-order kinetics at low substrate concentrations (i.e., $S<<K$) with the resulting first-order rate constant being equal to k/K. The Monod model is statistically superior to both the zero- and first-order models in all cases because of the additional regressable parameter K, which gives it greater flexibility in fitting any set of experimental data.

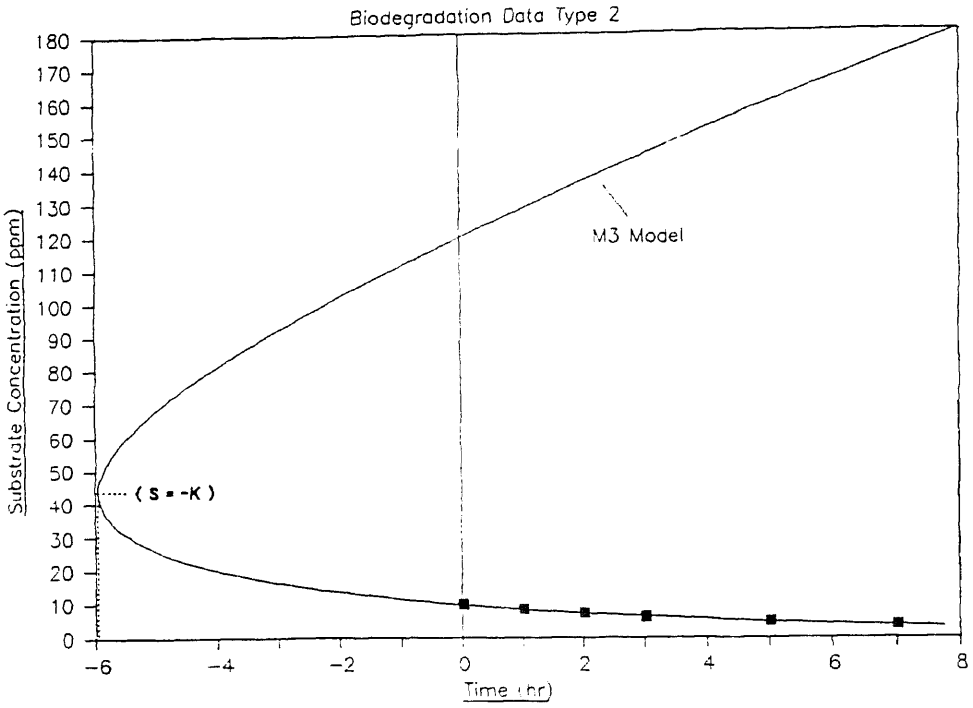
While the Monod model is inherently better at minimizing $\Sigma(t-tcalc)^2$, it does not necessarily mean that it better represents reality. The Monod model may incorrectly alter the curvature in otherwise purely first-order data (or similarly for zero-order data) by overfitting; an extreme example of overfitting is the manner in which an nth-order polynomial will fit a smooth curve through every data point even though the actual curve would not because of some degree of inherent experimental error in the data. This effect, however, is typically so slight for the case of the Monod model that it is negligible, especially for data with minimal experimental error. The more notable problem with the Monod model for first-order data is the possibility of regression yielding negative values for both kinetic rate constants k and K (refer to page E-65). Linear regression will yield negative values for the Monod models for all cases where S is observed

to drop at a greater than first-order rate, and positive values when the drop is less than or equal to first-order. For any experimentally measured first-order data, there is an approximately equal probability of regression yielding either both negative rate constants or both positive, depending on whether the scatter in the data can be interpreted as making the overall set greater than or less than first order, respectively.

Negative rate constants have no physical meaning and consequently invalidate any theoretical basis in the Monod models. Furthermore, practical use of the model is limited by the fact that -dS/dt becomes indeterminate when S equals the absolute value of K. This problem is displayed graphically in Figure 17 which shows an expanded version of the M3 curve. This regressed curve doubles back on itself at a value of S equal to the absolute value of K. A comparison of Figure 17 (k and K both negative) with Figure 7 (k positive and K negative) shows them to be, in effect, mirror images of one another relative to the ordinate.

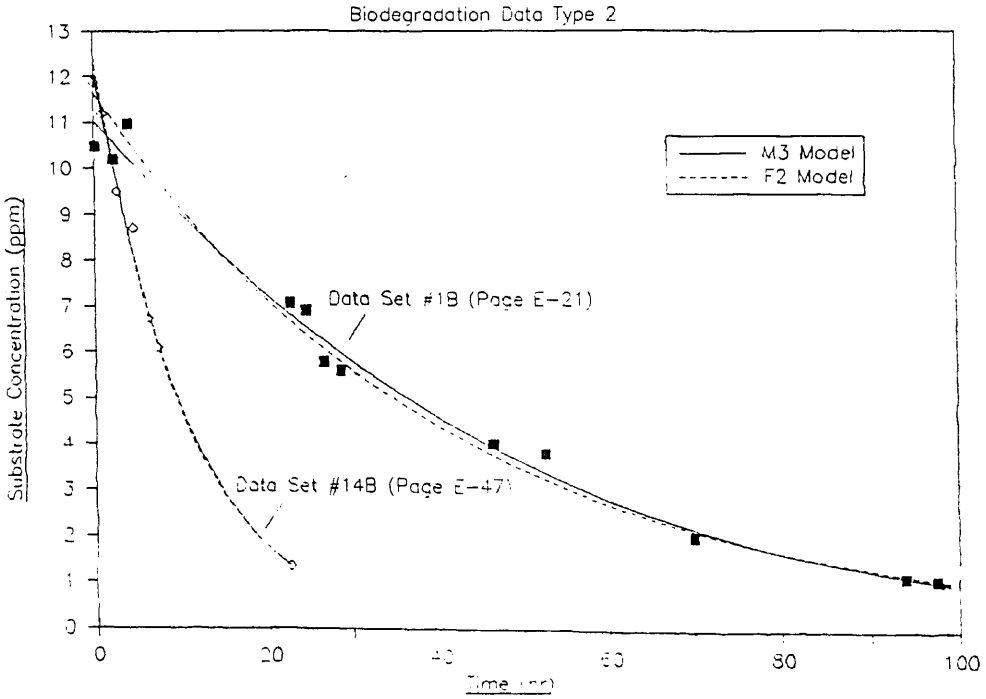
The first-order models are statistically only slightly inferior to the corresponding Monod models for the data set on page E-65, while Figures 15 and 16 show both F1 and F2 to well represent the data. The first-order models are technically sound in that they always yield positive rate constants for type 2 data and, as such, are generally preferred over the Monod models for this application.

Figure 17



Source : Naik Thesis (data set #38) ; refer to page E-65

Figure 18



Source : Gonnabathula Thesis (data sets #18 &14B) ; refer to pages E-21 & 47

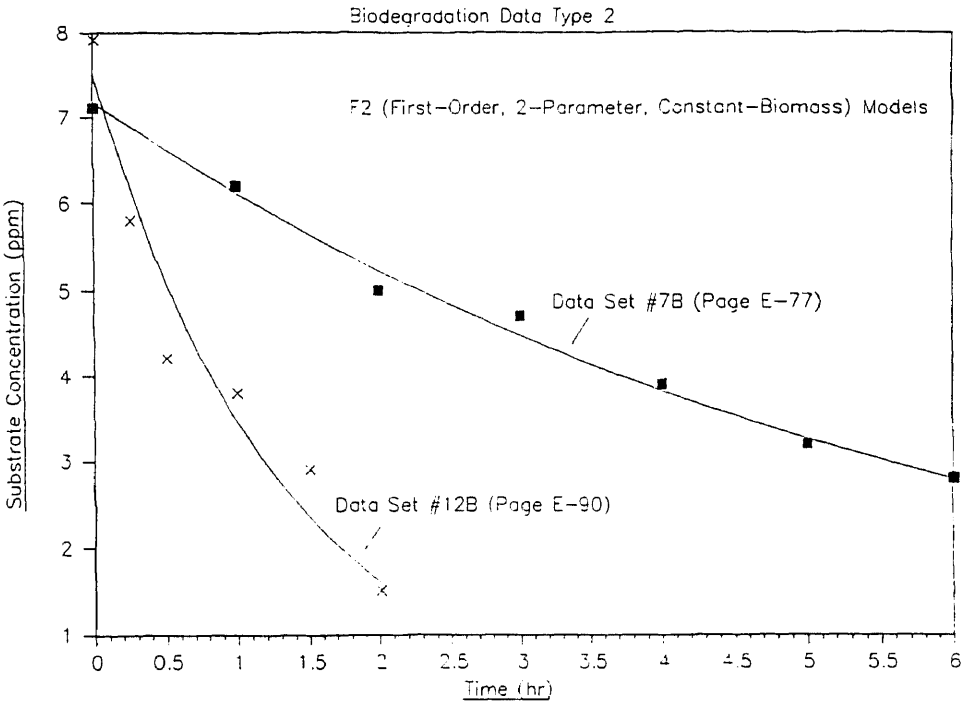
F2 is preferred to F1 because of its inherent ability to result in statistically better fits.

The zero-order, constant-biomass models are inappropriate for the above data because of their inherent inability to represent the necessary curvature which, in turn, accounts for them being the statitically worst of the group studied. Their inadequacy for modelling type 2 data is further magnified when extrapolating below the range of S used to regress them.

Figure 18 presents two more data sets of the second biodegradation data type with the regressed M3 and F2 curves shown for both cases. Both sets are for systems with low values of S/B and they exhibit a slightly increased amount of scatter vs. the set shown in Figure 15. Statistically and visually the models from all three sets perform comparably. The only notable difference between these two sets and the previous one is that the scatter in the former two is such that the Monod models interpret the biodegradation rates as being slightly less than first-order, thereby resulting in the regression of positive values of k and K for both data sets.

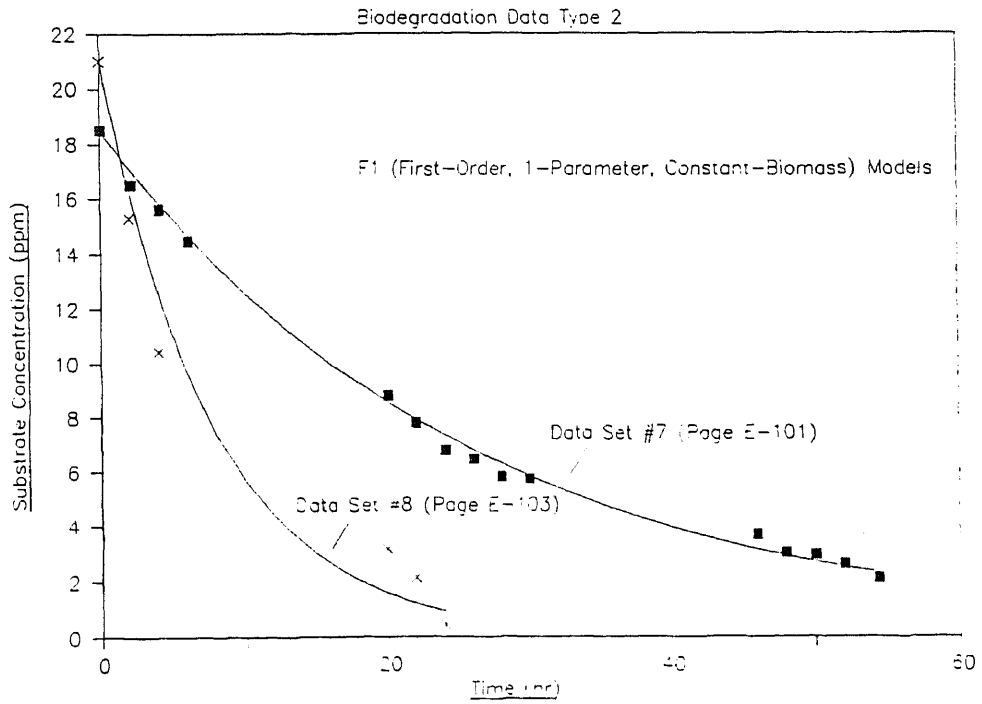
Figure 19 graphically presents the regressed F2 curves for the data sets shown on pages E-77 and E-90. Both of these sets are for the same substrate (i.e., nitrobenzene) but different activated sludge systems. The latter system uses a phenol-acclimated sludge (vs.

Figure 19



Source : Naik Thesis (data sets #7B & #12B) ; refer to pages E-77 & 90

Figure 20



Source : Pak Thesis (data sets #7 & #8) ; refer to pages E-101 & 103

an unacclimated sludge in the former) which accounts for its increased biodegradation activity as reflected in the notably higher first-order rate constants (i.e., k(F2) of 0.77/hr vs. 0.16/hr). Both of these sets exhibit increased scatter as compared to the previous three sets shown, resulting in statistically less significant differences between all of the models studied (compare $\Sigma(t\text{-}tcalc)^2$ on pages E-77 and E-90). It should be noted that, for the data set shown on page E-90, M3 regresses positive rate constants while M2 yields negative values. This is the combined result of the specific scatter in the data set and the relaxed restriction of So=S(t=0) for the M3 model. The M3 model has no real advantage over the M2 model in terms of regressing positive rate constants. An equal probability exists for the above situation to be reversed (i.e., positive k(M2) and K(M2) and negative k(M3) and K(M3)) depending primarily on the specific orientation of the data scatter.

Figure 20 presents two different sets of data for the same substrate/culture system (i.e., 2-chlorophenol/unacclimated sludge) along with the corresponding regressed F1 curves. The regression analysis results for the two sets are presented on pages E-101 and E-103. Whereas Pak designated both activated sludges as "unacclimated", the data set shown on page E-103 actually used the sludge from the set shown on page E-101. As a result of the sludge's previous exposure to the substrate, it had become partially acclimated accounting for the observed ca. three-fold increase in biodegradation rate (i.e., k(F1) of

0.13/hr vs. 0.038/hr). This example illustrates the importance of properly characterizing and quantifying the biocatalyst system in order to obtain usable kinetic data and, hence, applicable models.

The data set from page E-101 (shown graphically in Figure 20) was accompanied by biomass measurements facilitating the regression analysis shown on page E-102. The variable-biomass models yielded results comparable to the corresponding lower-parameter, constant-biomass models for the following reasons: (1) no variable-biomass effect was evident in the raw S vs. t data, and (2) the measured value of B represented the "total" microbial mass, and not the "viable" biomass, which resulted in B being so high relative to S that it was effectively constant over the range considered (i.e., based on the values of Bo and Yc, B increases by only 11% during the experiment). It should be noted that the values of Bo and Yc used are very suspect. A value of Yc greater than 1 can only be explained by either unaccounted-for substrate utilization or inaccurate B measurements. The latter is more than likely the case in this situation.

The regression results on pages E-101 and E-102 show that M2, M3 and MV all yield negative values for both k (or ko) and K because of an apparent greater-than-first-order drop. In general, MV will yield negative values for k and K in the same cases as the M2 model, providing Yc is positive. If Yc were negative, however, MV could regress positive values of both k and K in situations where the

constant-biomass versions do not. The effect of the negative Yc is to allow MV to fit a greater-than-first-order drop with positive rate constants; the more negative Yc is, the higher the drop that MV can fit with positive rate constants. The problem with this, however, is that a negative value for the substrate-specific parameter, Yc, is theoretically invalid. As substrate is consumed, a portion of the substrate is utilized by the "viable" biomass for growth, thereby always resulting in positive values of Yc.

In addition to the 7 data sets discussed thus far in this subsection, 2 more of the 124 mixed-culture data sets evaluated in this thesis have been classified as type 2 (refer to Figure 21). Both of these sets were extracted from the open literature. Neither author reported analytical accuracy (Lyons did, however, indicate reproducibility by performing measurements in triplicate and reporting mean values of S with calculated standard deviations), adequate biomass data (Lyons reported none while Wong's data was insufficient for determining Bo and Yc for variable-biomass modelling purposes), nor performed any kinetic analyses. Both studies were more interested in qualitative assessment and relative rates of biodegradation than generating data useful for engineering design purposes. Lyons' data set showed little scatter and yielded positive values of k and K for both M2 and M3 while Wong's data set exhibited significant scatter and yielded negative values of k and K for both M2 and M3. The scarcity of data points in the latter case, along with the apparent high degree of experimental

Figure 21

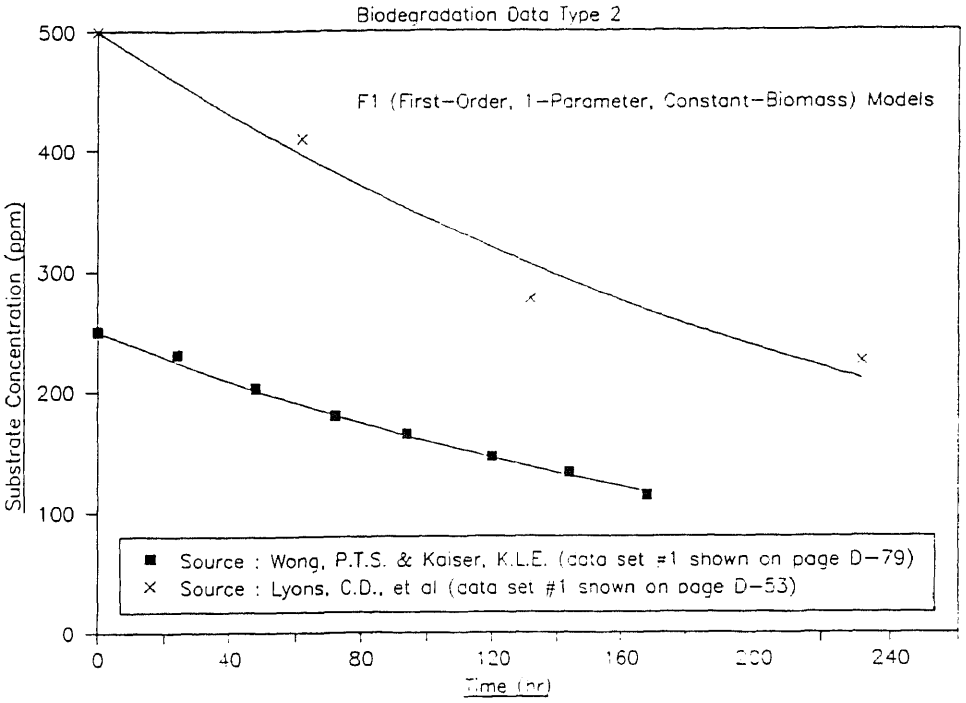
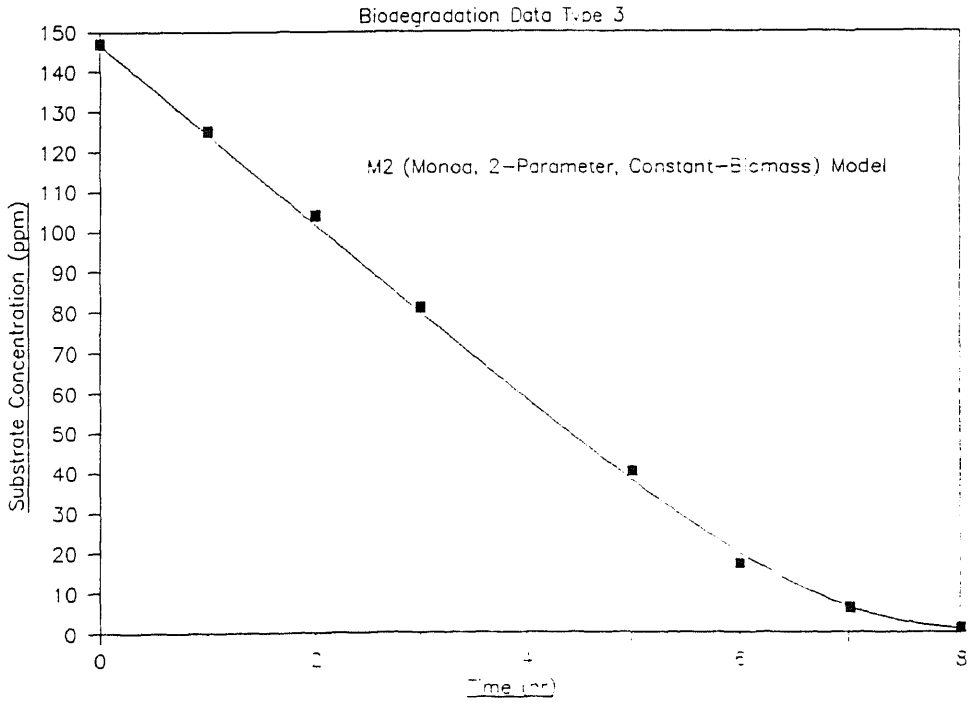


Figure 22



Source : Steger, V.W. & Tucker, E.S. (data set #2 shown on page D-69)

uncertainty makes model differentiation extremely difficult.

In order for the data shown in Figure 21 to have been of practical use to other scientists and engineers, the authors should have done the following: (1) reported the analytical accuracy of S values, (2) provided accurate measurement of "viable" biomass concentration, as well as a taxonomic definition or history of the culture, and (3) measured more than four S vs t data points. Wong did, however, to his credit eliminate abiotic effects (i.e., adsorption and stripping) from the S vs t data.

6.1.3 Data Type 3 (Monod, Constant Biomass)

Of the 124 mixed-culture, batch-reactor, raw aerobic biodegradation data sets evaluated in this thesis, 24 were categorized as type 3 or the Monod, constant-biomass type (refer to Figure 22). These sets are intermediate in order between zero and one. Some sets are mostly zero-order with a switch to the first-order regime at lower values of S, while others are mostly first-order. Data sets spanning the entire range of zero- to first-order are present. Both the zero- and first-order models are inappropriate for representing data of this type. The behavior of the zero-order models are analogous to that described in Section 6.1.2 for the fitting of first-order data, although the inadequacies are not as extreme, especially for the cases where the data sets are mostly in the zero-order realm. The same goes for the behavior of the first-order models being analogous to that described in

Section 6.1.1 in the fitting of zero-order data, with the inadequacies becoming less evident as the reaction order approaches one.

Figure 22 shows the data set from page D-69 to be well represented by the M2 model. The data has little scatter accounting for M3 being statistically only marginally better than M2. The other models are significantly worse. The data is basically zero-order down to an S value of ca. 40 ppm, at which point the transition to first order begins to take place. The transition from the zero- to the first-order regimes varies from experiment to experiment depending upon: (1) substrate type, (2) biomass type (i.e., concentration and composition), and (3) a myriad of other environmental conditions such as temperature and pH. It is apparent based on the above that prediction of biodegradation data type from the order of magnitude of S alone is not feasible.

The data set shown in Figure 22 was extracted from the open literature. Saeger and Tucker did not report analytical accuracy, measure biomass data, nor perform any kinetic analyses. Whereas non-biodegradation mechanisms (i.e., chemical oxidation and volatilization) were determined to be negligible, and whereas very little data scatter is apparent, the data presented in Figure 22 are of little use for design purposes without a quantitative measure of the "viable" biomass concentration.

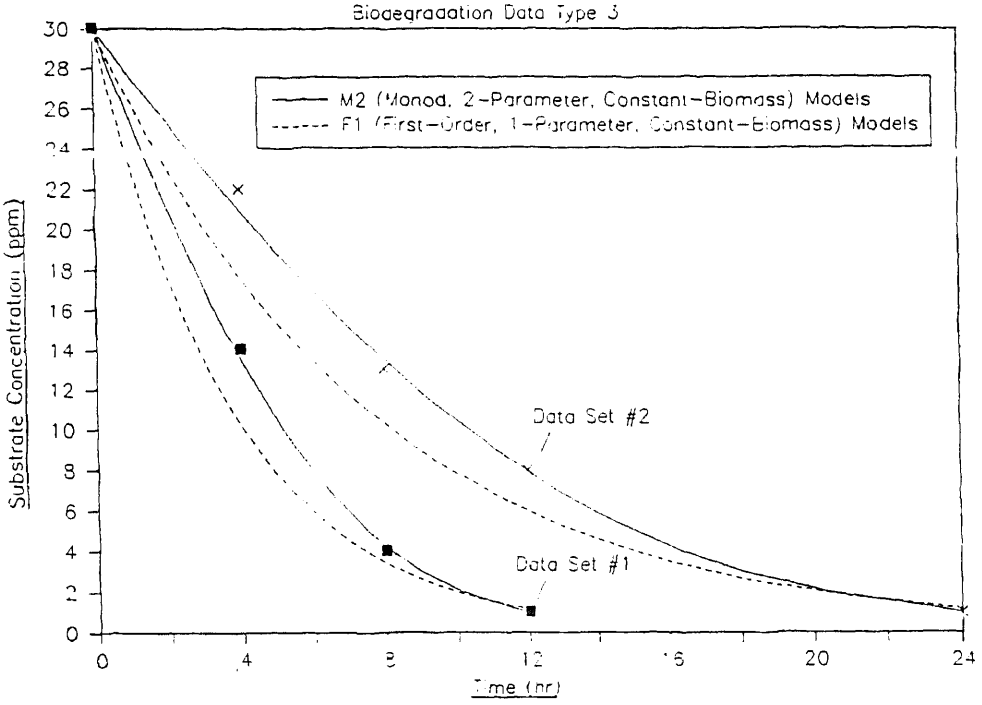
Figure 23 presents two data sets of biodegradation type 3, both of which were experimentally measured by Sayler, et al. In the article, the authors stated that the experiments were not well designed to determine reaction order. The data sets were said to be suggestive of first order, although the possibility of fractional-order kinetics was not ruled out. Even after the authors' expression of their awareness of their uncertainty with respect to reaction order, they incorrectly modelled and presented the kinetics as first-order. Figure 23 graphically shows (as the tabulations on pages D-70 and D-71 statistically do) that the data sets are clearly less than first order. As a side note, the first-order rate constants presented by Sayler, et al., are in agreement with those determined in this thesis (refer to Table 3 below).

Table 3

Regressed First-Order Rate Constants for Data Sets #1 and #2 on Pages D-70 and 71 (Source: Sayler, et al.)

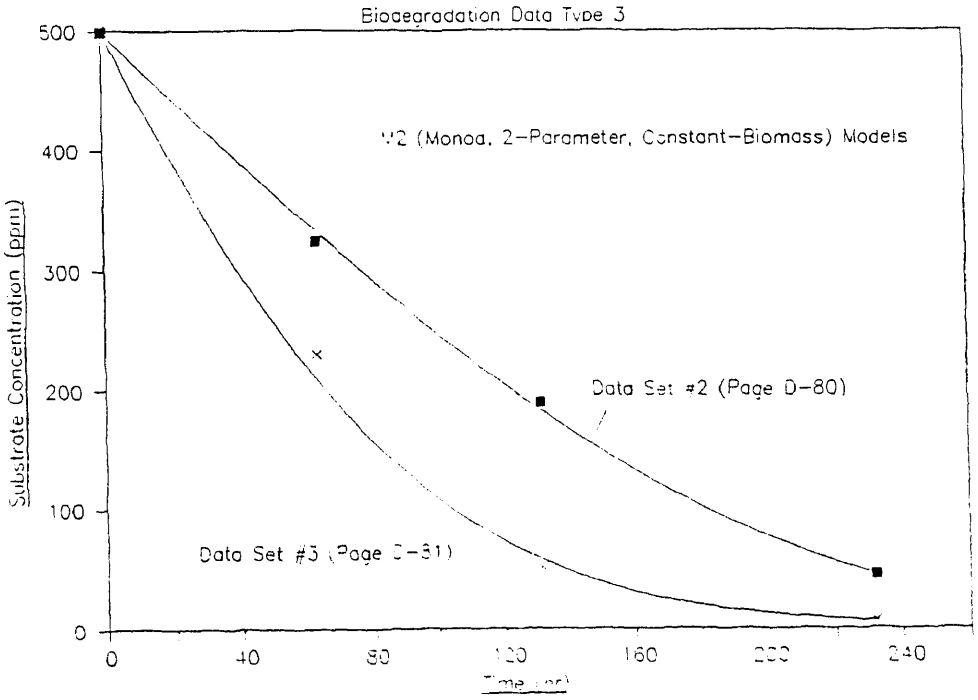
Data Set	Regressed Literature Value of k(1/hr)	Regressed Thesis Value of k(1/hr) k(F1)	k(F2)
#1	0.28	0.270	0.291
#2	0.14	0.134	0.147

Figure 23



Source : Sayler, G.S., et al (data sets #1 & #2 shown on pages D-70 & 71)

Figure 24



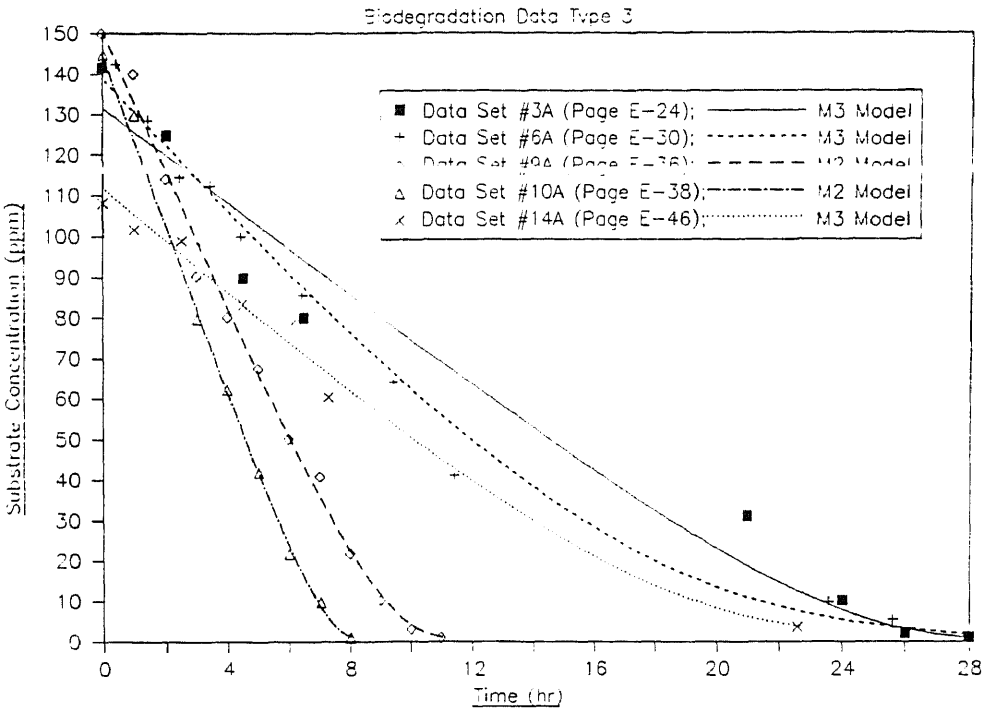
Source : Wong, P.T.S. & Kaiser, K.L.E. (data sets #2 & #3 on pages D-80 & 81)

While the data sets presented in Figure 23 have minimal scatter and are well represented by the Monod models, they are of no practical use for design purposes due to the lack of qualitative and quantitative information about the activated sludge system. No difference between the sludge used in the two data sets was indicated by the authors, yet a two-fold difference in biodegradation rate was observed for the two purportedly identical systems and conditions.

Figure 24 presents two more data sets of biodegradation type 3, both of which were experimentally measured by Wong and Kaiser. These two sets were extracted from the same article as that data set shown in Figure 21 and the same general comments made on pages 48 and 50 for that set are applicable here except for the fact that it was interpreted as type 2 data (note: all three sets are for different substrates and, as a result, have different biodegradation rates).

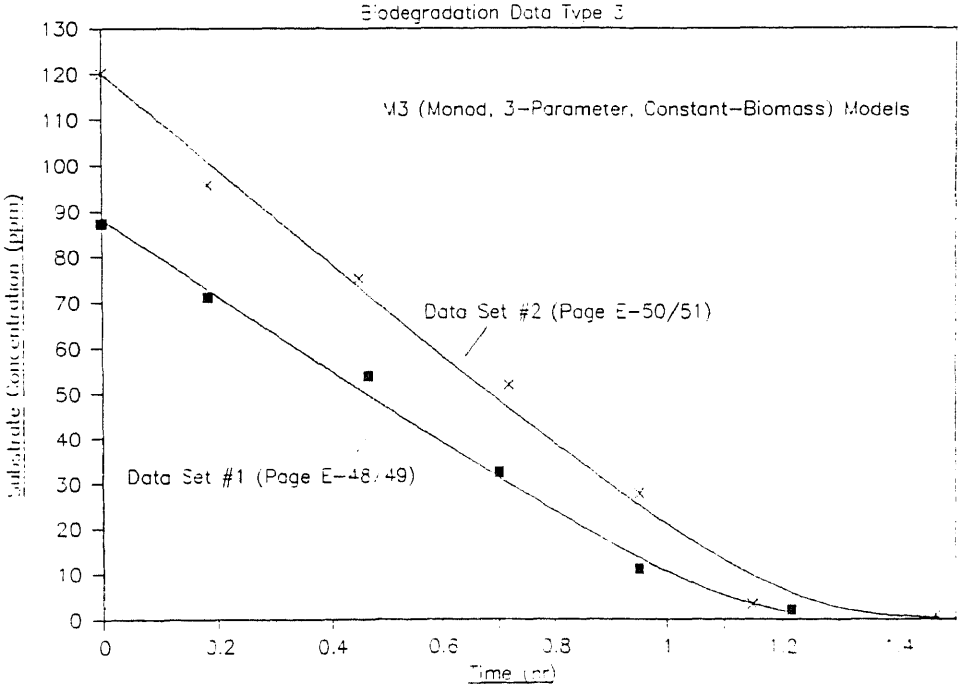
Figure 25 graphically presents five data sets from Gonnabathula's thesis which are for the same substrate (i.e., phenol) and are all of the same biodegradation type (i.e., type 3). All five sets were measured under virtually identical experimental conditions (e.g., NH_3 content, MLSS level and temperature) except for co-substrate type. Table 4 summarizes below the Monod rate constants for each set and specifies the co-substrate used in each case. Significant variability between the results for the same substrate and conditions,

Figure 25



Source : Gonnabathula Thesis

Figure 26



Source : McMullen Thesis (data sets #1 & #2 on pages E-48/49 & 50/51)

even for the cases with the same co-substrate, is apparent. In each of the five sets shown in Figure 25, not only does the rate of the zero-order drop vary (as reflected in the k(M3) values varying ca. 400% from 6.18 to 23.29), but so does the point at which transition to first-order kinetics begins (as reflected in the K(M3) values varying ca. 400% from 8.50 to 37.12). These results differ from one another because of subtle differences in the activated sludges which were not sufficiently represented by crude MLSS measurements. Knowledge of the biocatalyst amount, type and history is critical to the measurement and utilization of biodegradation data.

Table 4

Regressed M3 Model Rate Constants for Phenol as Substrate in Activated Sludge (Data Source: Gonnabathula Thesis)

Data Set	Co-Substrate	k(M3), ppm/hr	K(M3), ppm
#3A	2,6-dichlorophenol	6.18	8.76
#6A	2-chlorophenol	10.61	37.12
#9A	2-chlorophenol	19.07	11.93
#10A	2-chlorophenol	23.29	8.50
#14A	Nitrobenzene	7.59	18.36

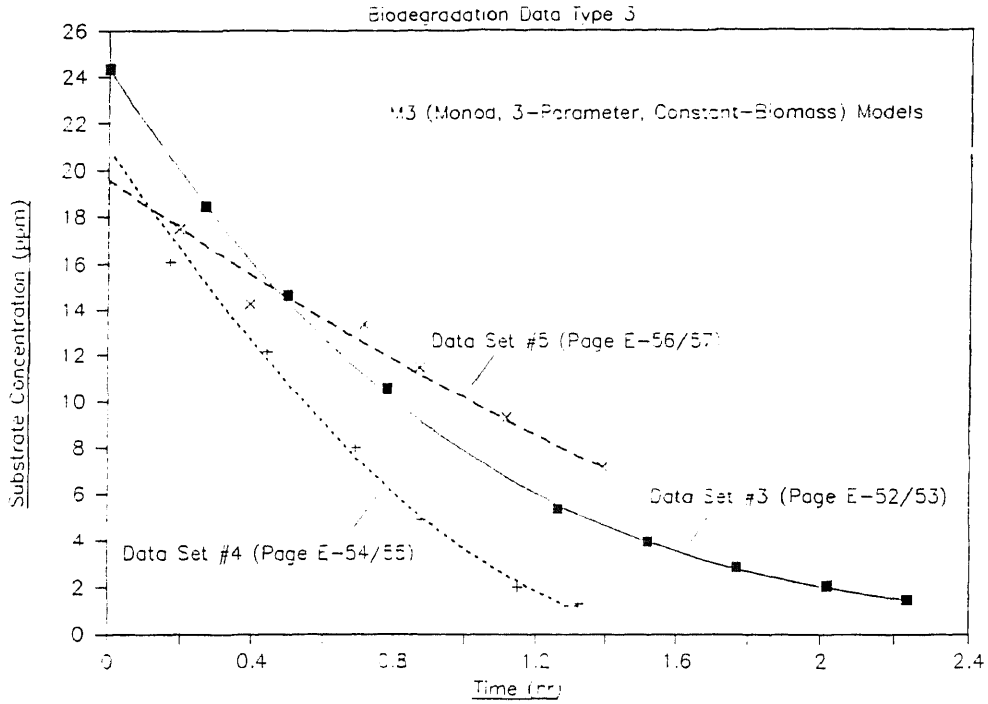
Figure 26 presents two other data sets of biodegradation type 3 for the substrate phenol (this time as the sole carbon source) in activated sludge. The degradation is much more rapid in these two sets as compared to those shown in Figure 25, which may either be due to inhibitory effects of the co-substrates used by Gonnabathula, or just to inherent differences in the activated sludges. It should be noted that MLSS measurements by McMullen were ca. 50% higher for data set #1 vs. data set #2 (refer to pages E-49 and E-51, respectively), yet the latter set exhibited more rapid biodegradation. The reason for this is that the sludge from the first set was used as inoculum for the second; partial acclimation had occurred with growth of the substrate-specific bacteria while the bulk of the biomass (being non-viable) decreased, resulting in lower MLSS values. This further exemplifies the inadequacy of MLSS measurement as a gauge of biocatalyst activity.

Pages E-49 and E-51 summarize the regression results for variable-biomass models for the two data sets shown in Figure 26. The variable-biomass models are no better than the constant-biomass versions for this data type because no variable-biomass effects are evident; the variable-biomass effects present in the data sets discussed in this subsection are negligible relative to the experimental uncertainties in the data. Furthermore, the values of Bo and Yc are based on crude MLSS measurements causing the variable-biomass models to yield results of questionable validity. Page E-49 shows the substrate-specific parameter Yc to be -0.617, which is not theoretically valid.

Gonnabathula also provided MLSS measurements for all of his biodegradation data sets as McMullen did. Variable-biomass models were not evaluated in the former case, however, because of the additional complication of co-substrates being present. Yc is a substrate-specific parameter and no reliable method is available to calculate it from bulk mixture measurements. Yc can only be accurately determined for single-substrate systems. Application of Yc values determined in this manner to multiple substrate systems may not necessarily be valid due to potential interactive effects.

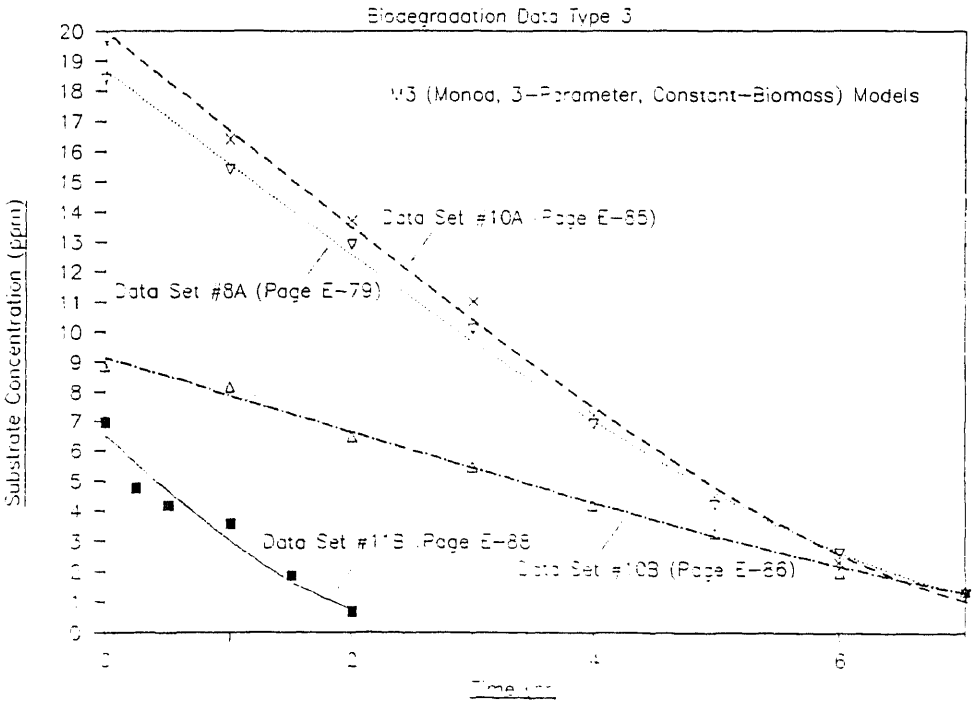
Figure 27 graphically presents three data sets for 2-chlorophenol as sole substrate in activated sludge, as measured by McMullen under virtually the same conditions (refer to pages E-52 through E-57). Table 5 below again shows the significant variation, in terms of the regressed rate constants, between repeated experiments run under presumedly identical conditions. Better definition and control of the reaction system in terms of key parameters (e.g., biomass type/amount, nutrients, temperature, agitation, etc.) are required to obtain reliable data and models. Based on the observed trend in the tabulated data and the fact that the inoculum to each set is the activated sludge from the previous set, it appears that the viable biomass concentration is dropping (along with the total biomass concentration, as indicated by the calculated negative values of Yc), possibly due to some inhibitory or toxic effect associated with utilization of the substrate.

Figure 27



Source : McMullen Thesis (data sets #3,#4 & #5 on pages E-52/53, 54/55 & 56/57)

Figure 28



Source : Naik Thesis (data sets #8A,#10A,#10B & #11B on pages E-79,85,86 & 88)

Table 5

Regressed M3 Model Rate Constants for 2-Chlorophenol as Substrate in Activated Sludge (Data Source: McMullen Thesis)

Data Set	k(M3), ppm/min.	K(M3), ppm
#3	1.14	45.4
#4	0.52	9.1
#5	0.27	10.6

Four more data sets of biodegradation type 3 are presented in Figure 28. All four were extracted from Naik's thesis and each involved simultaneous biodegradation of two co-substrates. Variable-biomass models were not evaluated (although no improvement would be expected over the constant-biomass versions for data of type 3) because of the inability to calculate Yc for a specific substrate from nonsubstrate-specific bacterial measurements. Data sets #8A and #10A are duplicate experiments on 2-chlorophenol substrate with apparently good reproducibility being achieved. Data sets #10B and #11B are identical experiments (for nitrobenzene substrate) except for the sludges; the former used unacclimated sludge while the latter used phenol-acclimated sludge which, in turn, accounted for the notably higher biodegradation rate.

In addition to the 19 data sets discussed thus far in this subsection, Figures 29 through 32 present the 5 remaining sets studied in this thesis which were classified as biodegradation type 3.

Figure 29 shows two sets of data for the same system (i.e., 2,6-dichlorophenol in MLSS) at comparable conditions from two different sources (i.e., Pak and Gonnabathula) yielding reproducible results. While the two curves overlap reasonably well, the regressed values of k(M3) and K(M3) for the two data sets as shown on pages E-23 and E-95 still differ appreciably, specifically the K(M3) value. This demonstrates the mutual sensitivity of k and K in the Monod models to slight changes in the data as compared to the single rate-constant models. It should be noted that both of these data sets exhibit significant scatter making model differentiation difficult (refer to the Σ(t-tcalc)^2 values on pages E-23 and E-95). Within the accuracy of the data, the zero- and first-order models (although statistically worse) cannot be discounted with any great confidence.

Figures 30 and 31 show two data sets that are well-represented by the M3 model. The data in Figure 30 was extracted from the open literature. As in most of the literature sources reviewed, the authors did not: (1) report analytical accuracy and (2) measure and characterize the biocatalyst. This makes the data presented of little use to others for design purposes. Taylor and Ribbons were more concerned with the study of the mechanism of metabolic breakdown of

Figure 29

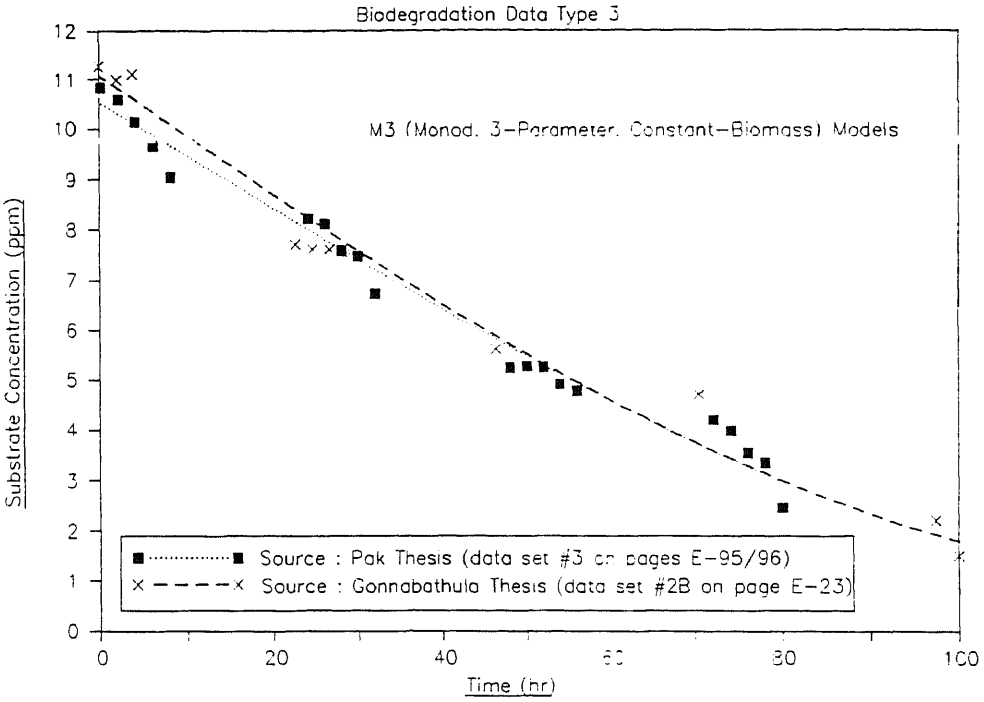
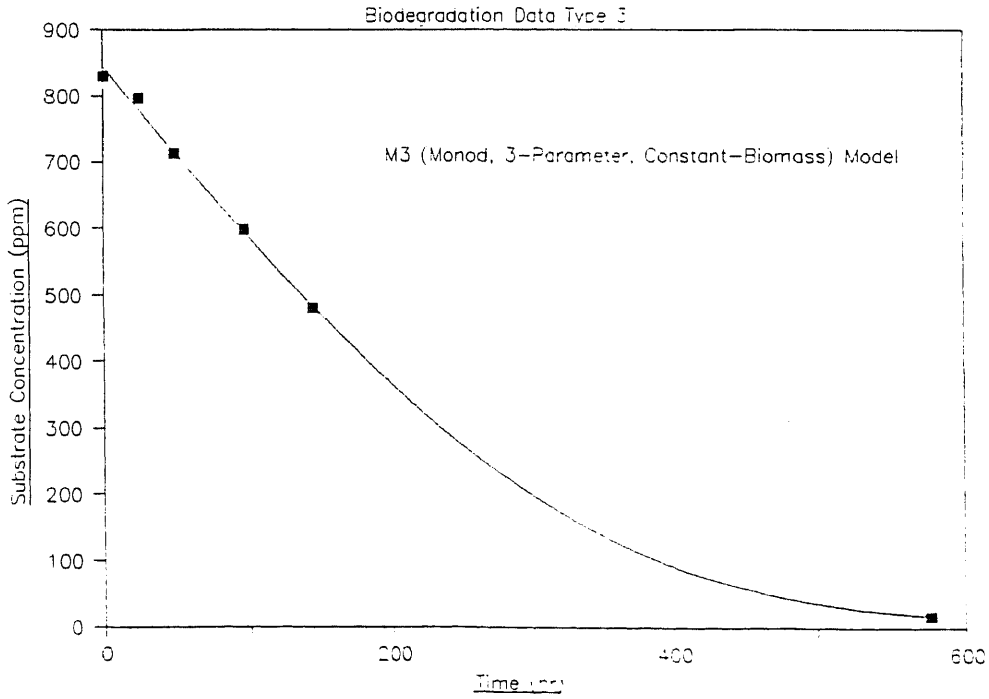
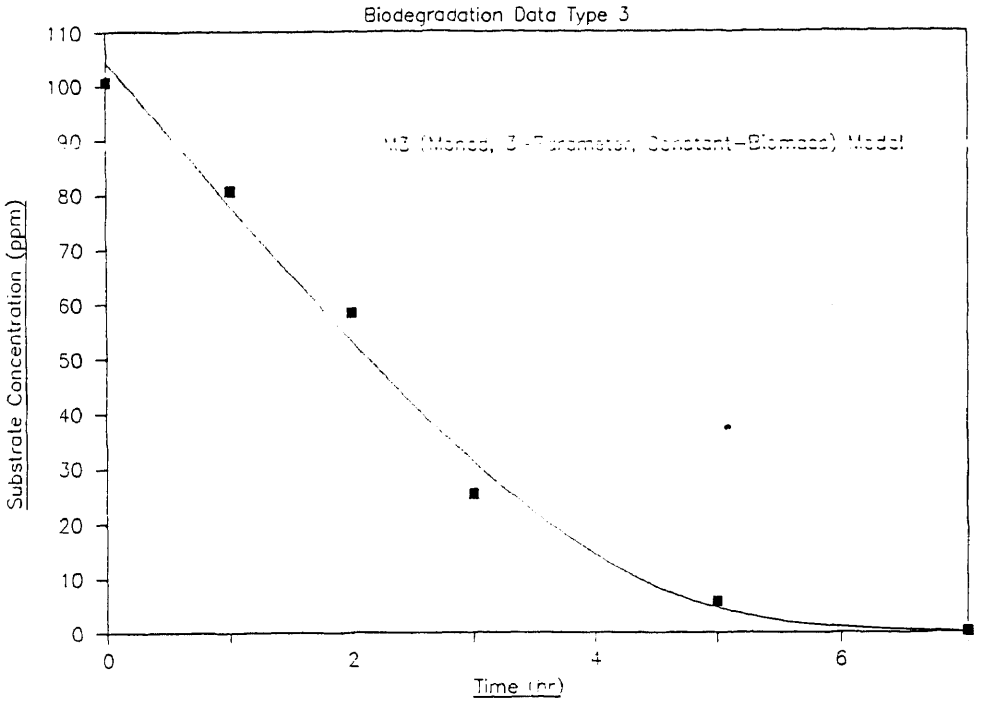


Figure 30



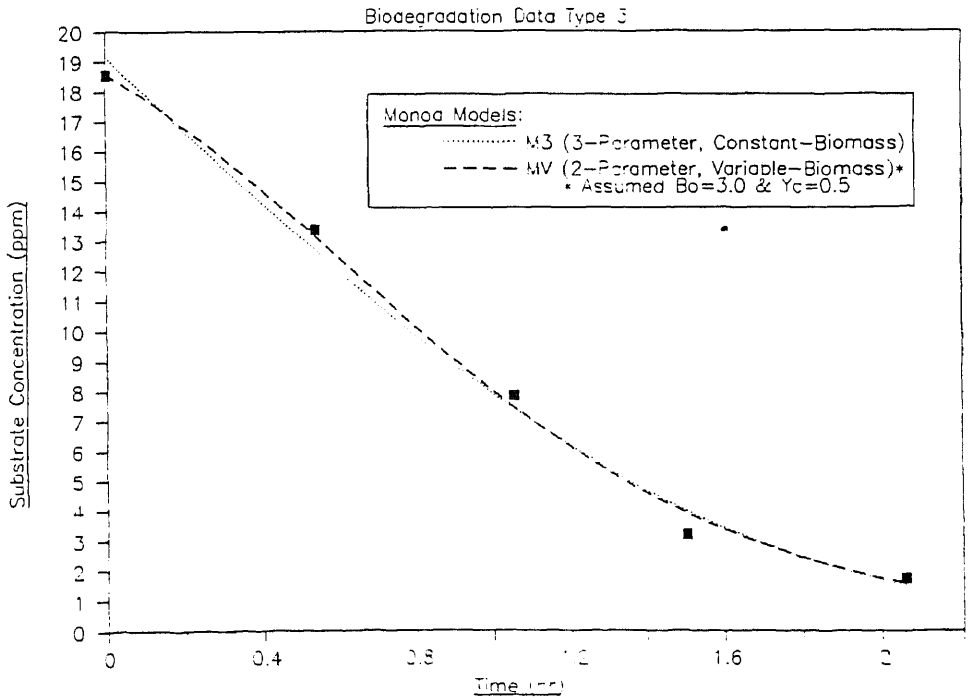
Source : Taylor, B.F. & Ribbons, D.W. (data set #3 shown on page D-78)

Figure 31



Source : Naik Thesis (data set #2A shown on page E-61)

Figure 32



Source : Pak Thesis (data set #6 shown on page E-100)

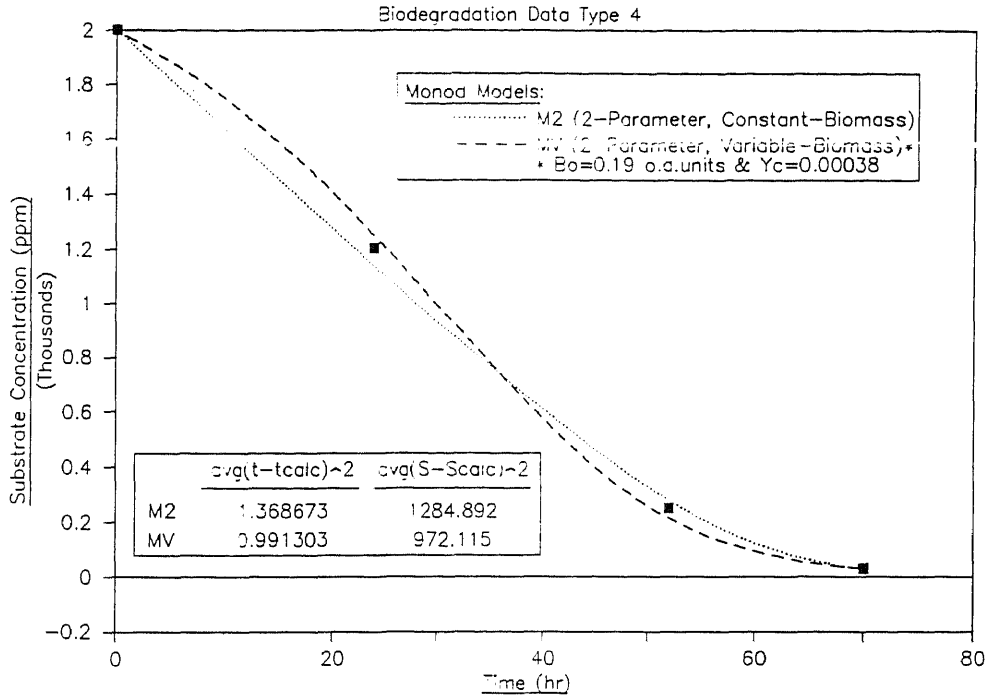
o-phthalic acid than with providing data for design. They performed no kinetic analysis of their data.

Figure 32 shows a data set which is well-represented by the M3 model to be better represented by the MV (Monod, 2-parameter, variable-biomass) model. Biomass data were not provided for this set and it is not sure whether MV is the correct interpretation of the data or whether it just happens to result in a better fit for the specific scatter present. The value of Yc used on Figure 32 was assumed to be 0.5 (considered a typical value for Yc) while the value of Bo was selected so as to minimize the value of $\Sigma(t\text{-}tcalc)^2$ (i.e., 0.004144 vs. 0.006372 for M3). It should be noted that, while lower values of Bo (i.e., <3.0) resulted in even lower values of $\Sigma(t\text{-}tcalc)^2$, they also resulted in the MV model regressing negative values for both ko and K.

6.1.4 Data Type 4 (Monod, Variable Biomass)

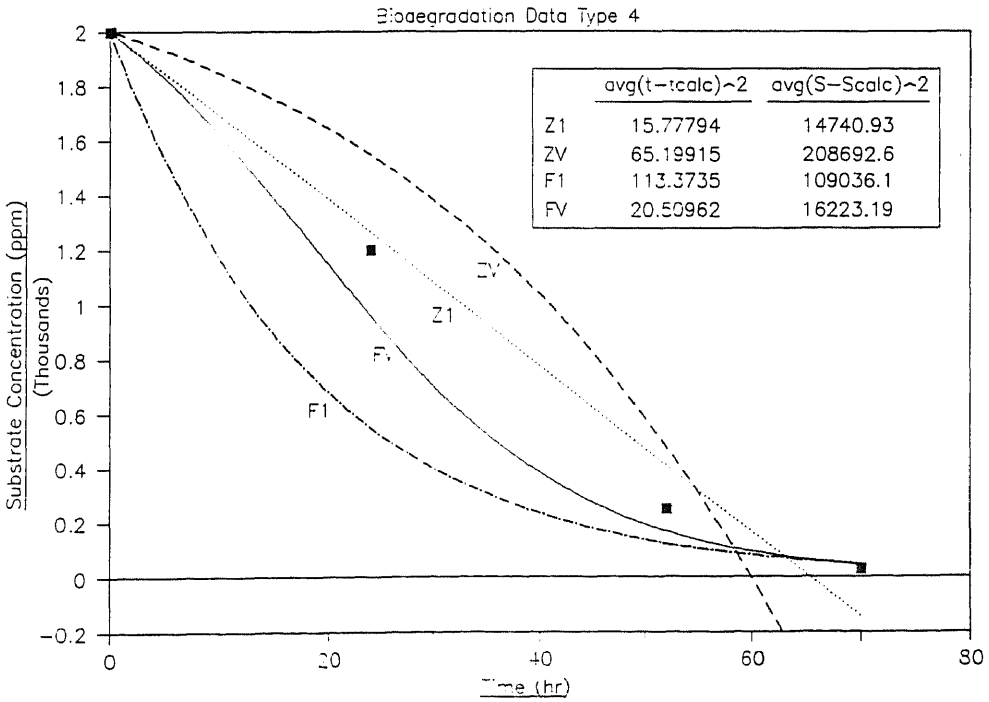
The next biodegradation data type to be discussed is the variable-biomass version of data type 3 which is well-represented by the MV (Monod, 2-parameter, variable-biomass) model as demonstrated in Figure 33 for the data set shown on page D-36. The data summary for the variable-biomass kinetic analysis of this set is not contained in the appendix, but the results are displayed graphically for each model (i.e., MV, ZV and FV) in Figures 33 and 34.

Figure 33



Source : Valendinov, A.N., et al (data set #3 shown on page D-36)

Figure 34



Source : Valendinov, A.N., et al (data set #3 shown on page D-36)

Ilyalendinov, et al, measured and presented the biomass data in optical density units as opposed to the more common concentration unit of ppm seen throughout this thesis; this accounts for the much lower numerical values of Bo and Yc. The units of Bo and Yc are not critical except to the extent that they are consistent with one another. The variable-biomass data presented by the authors are of better quality, even though only four data points were available, than any of the MLSS measurements discussed thus far (as demonstrated by the resulting good fit by the MV model in Figure 33). The bacterial cultures discussed previously were activated sludges, which by definition consist of a large, diverse group of bacterial species in a complex heterotrophic system. However, the culture used by Ilyalendinov, et al, consisted of a mixture of only two pure bacterial strains (i.e., B. cereus and P. aeruginosa) in a single-level trophic system. Because this mixed-culture system contained only two strains, both capable of utilizing the alpha-methylstyrene substrate (vs. an activated-sludge system where a high percentage of the bacterial strains are inactive/non-viable) in a single-trophic system (vs. a heterotrophic system where non-viable, non-bacterial microorganisms are present), this system resulted in more reliable predictions of Bo and Yc. These

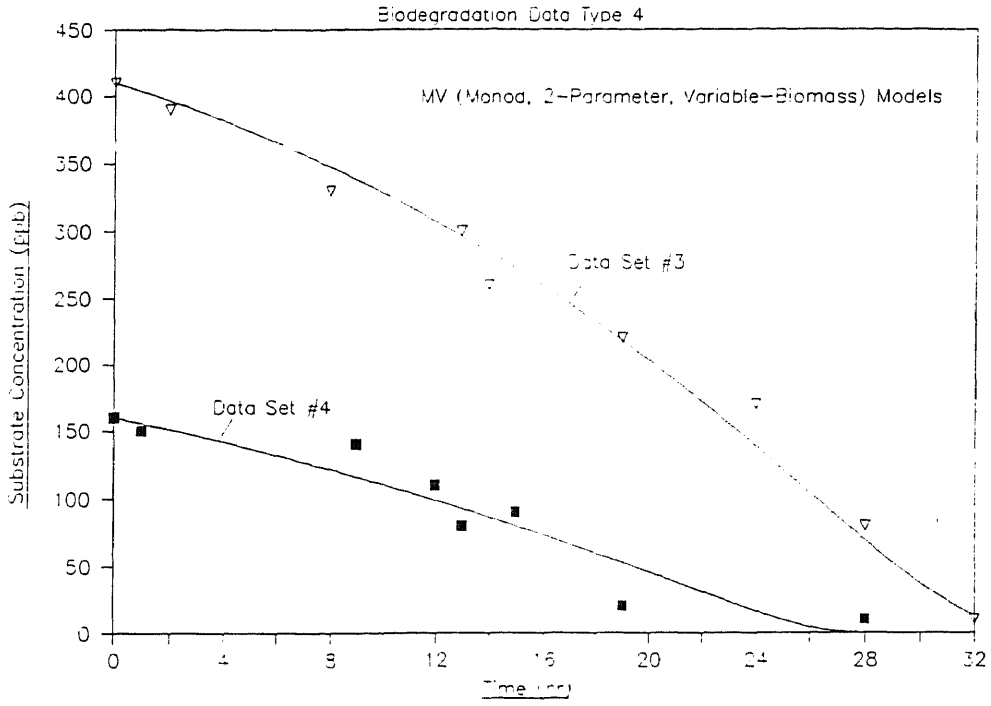
values, however, still suffer from the inaccuracies (although not nearly to as great an extent) related to the biomass measurement techniques which do not differentiate between living and dead cells. The MV model would have resulted in a better fit if a lesser variable-biomass effect had been predicted by Bo and Yc (i.e., if Bo were higher or Yc were lower, or a combination of both). The accuracy of Yc used here is more suspect than Bo based on the fact that Yc varied significantly (rather than remained constant as is a basic presumption of the variable-biomass models evaluated in this thesis) over the range of S covered. Variation of Yc with conversion has been noted elsewhere in the literature by Pirt[3] and Yang and Humphrey.[4] Yc varied here due to utilization of the substrate having encompassed the pre-exponential and declining-growth phases, and not just the exponential growth phase over which Yc should remain virtually constant.

Figure 33 shows MV to be statistically and visually the best of the models evaluated. The constant-biomass Monod models, however, are not unreasonable, even though B increases five-fold over the range of S covered. Considering that there are only four data points and that the authors did not report analytical accuracy (nor did they perform any kinetic analysis), M3 and M2 cannot be discounted with complete confidence as incorrect representations of the system.

Figure 34 shows the lower-parameter, constant-biomass versions of the zero- and first-order models along with the corresponding variable-biomass versions. None of the models are good for the data set shown. Because of the nature of Monod kinetics spanning the range from zero to first order, there will be instances where the type 4 data will be mostly zero order and, hence, will be reasonably well represented by ZV; analogously, the type 4 data may on occasion be mostly first order and, hence, will be well represented by FV. The extent to which the constant-biomass models are reasonable for such data depends on the extent to which B varies. The general characteristics of FV and ZV for typical type 4 data are visually demonstrated in Figure 34. A more detailed discussion of the characteristics of each of the variable-biomass models and their sensitivity to the parameters Bo and Yc will be provided later in this section.

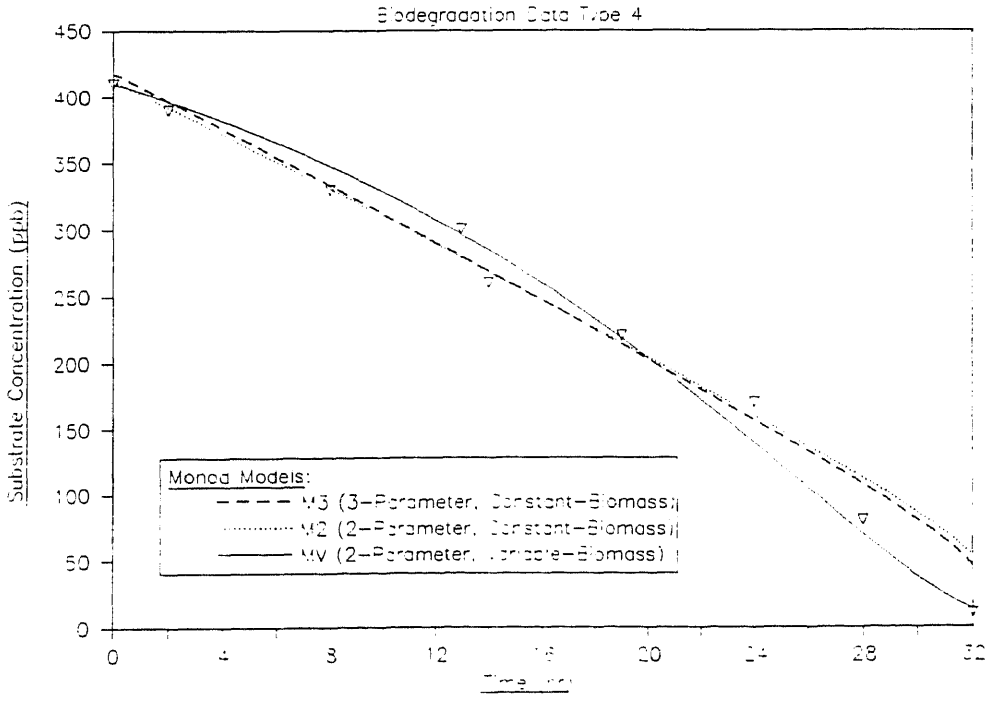
Figure 35 provides two data sets of type 4 for pentachlorophenol substrate in MLSS for two different values of So. The values for ko and K on pages D-46 and D-48 for the two sets are quite different. This difference in biodegradation rate is attributed by Klecka and Maier to substrate inhibition. They took this into account when they modelled the data by using the Haldane modification of the Monod equation:

Figure 35



Source : Klecka, G.M. & Maier, W.J. (data sets #3 & #4 on pages D-45 thru 48)

Figure 36



Source : Klecka, G.M. & Maier, W.J. data set #3 on pages D-45 & D-46)

$$-\frac{dS}{dt} = \frac{\mu B}{Yc}\left(\frac{S}{(K+S+S^2/K_I)}\right) \quad ; (1)$$

where,

$$k = \frac{\mu B}{Yc} = koB$$

μ = maximum bacterial growth rate

S^2/K_I = substrate inhibition term

K_I = substrate inhibition constant

They also incorporated an endogenous decay coefficient (k_D) within the biomass equation:

$$\frac{dB}{dt} = \frac{\mu B}{Yc}\left(\frac{S}{(K+S+S^2/K_I)}\right) - k_D B \quad ; (2)$$

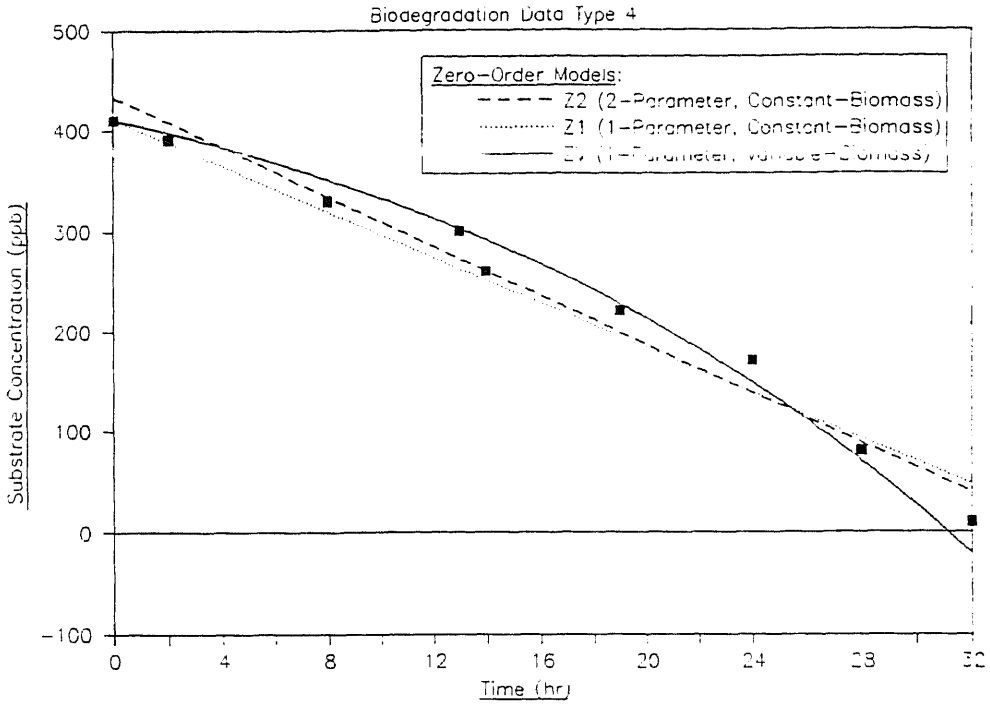
The inclusion of the substrate inhibition and endogenous decay terms (i.e., S^2/K_I and $k_D B$, respectively) results in a more complex model requiring determination of the kinetic parameters (i.e., μ, K, K_I, and Yc; k_D was assumed a constant value of 0.002 h^{-1} by the authors) through the use of numerical methods on a mainframe computer. Whereas this model better represents this specific system than the models evaluated in this thesis, its increased complexity reduces its utility as a general purpose tool.

For data set #3 shown graphically in Figure 35, the statistically best models of those evaluated in this thesis in terms of Σ(t-tcalc)^2 are, in order from best to worse (refer to pages D-45 and D-46): (1) M3, (2) M2, (3) MV, (4) ZV, (5) Z2, (6) Z1, (7) FV,

(8) F2, and (9) F1. While M3 and M2 are slightly better than MV in terms of $\Sigma(t\text{-}tcalc)^2$, they are much worse in terms of $\Sigma(S\text{-}Scalc)^2$ (refer to Figure 36). The MV model's performance is hindered somewhat by the questionable accuracy of B measurements. For higher values of Bo (i.e., 25 vs. 18.9 ppb) or lower values of Yc (i.e., 0.1 vs. 0.136), MV performs better than M3 and M2 in all respects. Furthermore, it should be noted that both M3 and M2 regress negative values for the kinetic parameter K due to the predominantly downward bend in the data. This is analogous to the situation discussed previously in Section 6.1.1 on pages 27-31 with respect to the cases in which the Monod (constant-biomass) models yield negative values of K for zero-order data. M3 and M2 will regress negative values of K for type 4 data in cases where the downward bend predominates versus the opposing first-order curvature. Depending on the given data set, M3 and M2 can both yield positive or negative values of K; it is also feasible that situations may arise where M3 and M2 will yield K values of opposite sign. Because the constant-biomass Monod models are unable to model the downward bend in type 4 data without the regression of negatives values for K, they are as a general rule inappropriate for type 4 data.

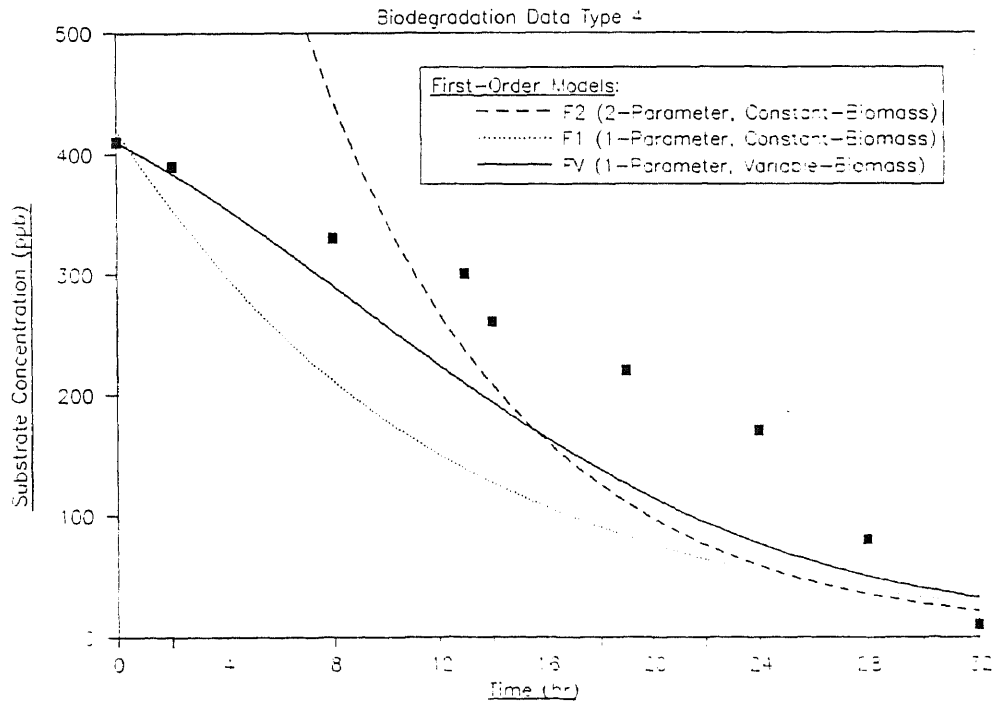
Figures 37 and 38 present all of the zero- and first-order models, respectively, for the same data set shown in Figure 36. In both cases, the variable-biomass curves are better than the corresponding constant-biomass models, but all are notably worse than the MV curve shown in Figure 36.

Figure 37



Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Figure 38

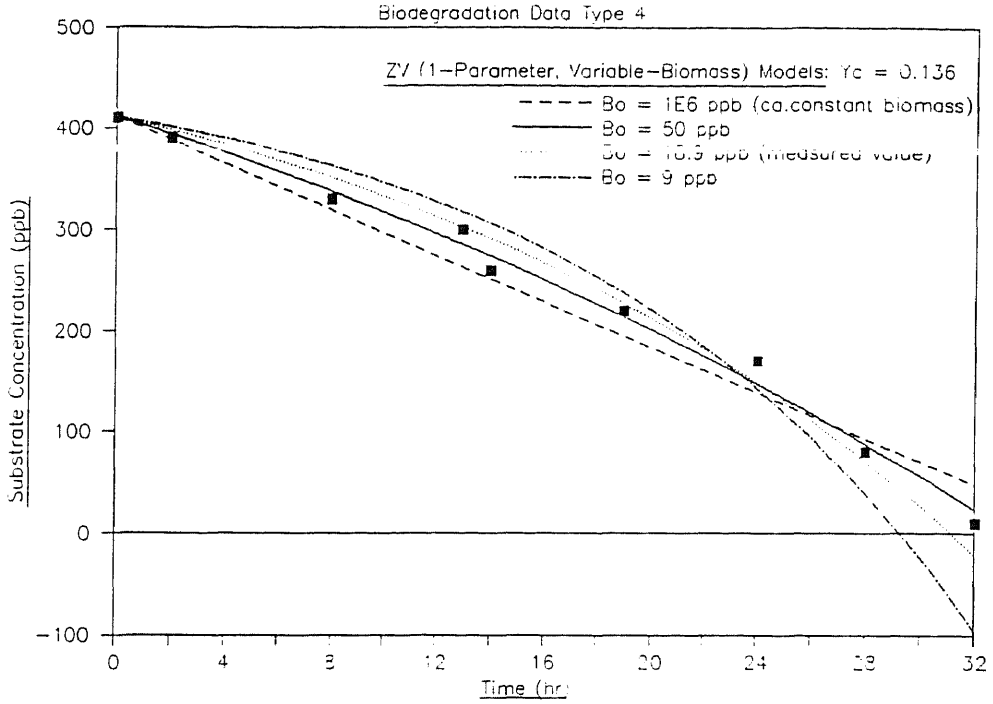


Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Whereas the constant-biomass, zero-order models are incapable of fitting any curvature (slope = dS/dt = constant = -k), Figure 37 shows that ZV does not have this restriction because of the assumption of exponential biomass growth (slope = dS/dt = -koBo*exp(koYct); this expression reduces to dS/dt = -koBo = -k when Yc=0 or, in other words, when constant-biomass conditions prevail). As in the constant-biomass case, the variable-biomass model predicts complete degradation after a finite period of time (i.e., x-intercept at t = (1/koYc)ln(1+YcSo/Bo)) beyond which negative values of S are predicted. It is because of the inability of ZV to model the inflection in type 4 data that it is inappropriate in virtually all cases, especially when extrapolating.

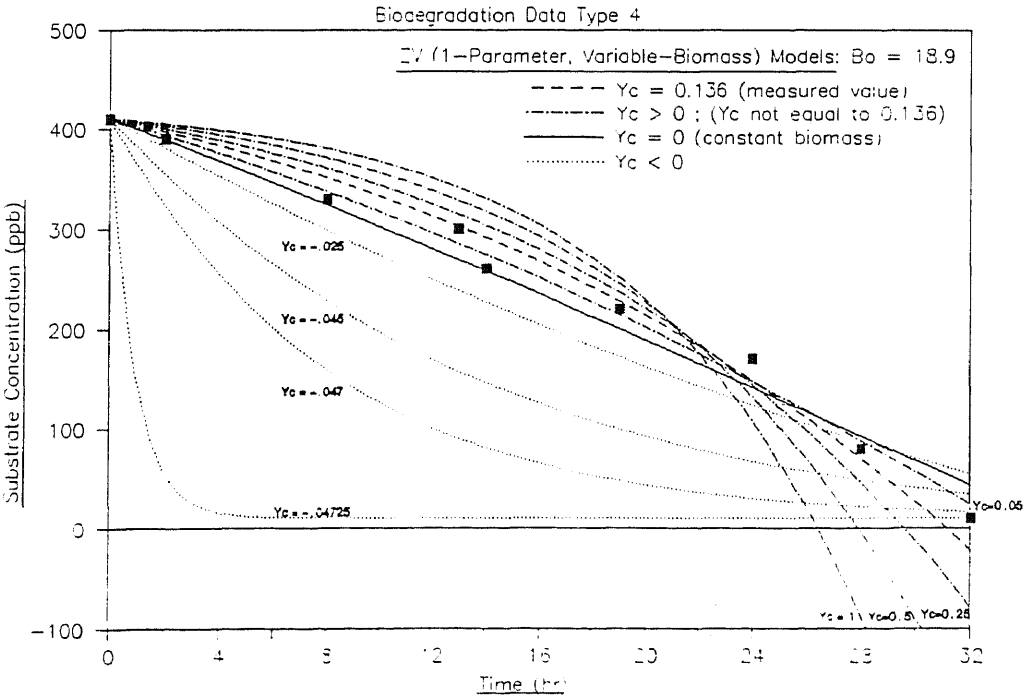
Figures 39 and 40 show the effects of the values of Bo and Yc, respectively, on the performance of the ZV model for the same data set presented in Figures 35 through 38. Bo is always a positive value with theoretical limits of 0 and 1,000,000 ppm. Figure 39 shows that ZV approaches constant-biomass behavior as Bo increases. As Bo decreases, the variable-biomass effect increases (i.e., the predicted initial biodegradation rate decreases, approaching the limit of 0, while the rate of change becomes more dramatic, approaching the limit of an almost vertical drop). Figure 39 shows that a much better fit of the data is obtained with the ZV model when a value of 50 ppb is used in place of the measured value of 18.9 ppb for Bo. This does not

Figure 39



Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Figure 40



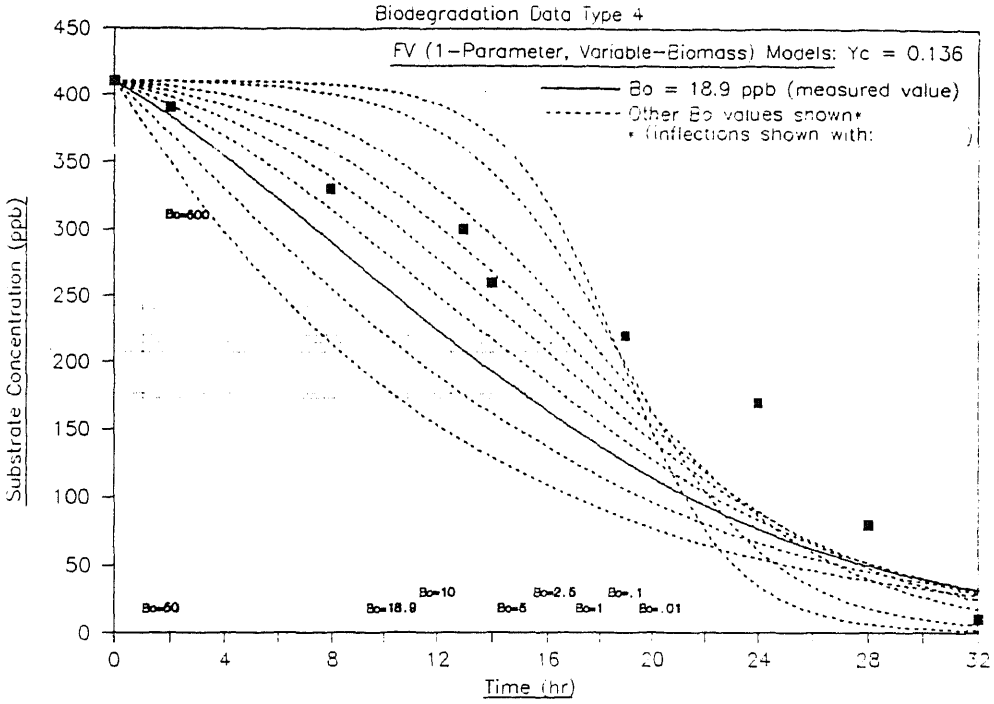
Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

necessarily mean, however, that the measured value of Bo is inaccurate. Rather, the value of Yc may be more suspect.

Figure 40 shows the effect of the value of Yc on the regressed ZV curves. Whereas Yc is typically expected to have values of between 0 and 1, negative values have in certain anomalous situations been observed to occur and they were therefore examined here, even if only for esoteric purposes. The higher the value of Yc, the greater the variable-biomass effect observed; constant-biomass behavior is approached as Yc approaches 0. As values of Yc drop below 0, the curvature of the ZV model is reversed resembling that of positive nth-order kinetics. ZV curves for negative values of Yc can be predicted only for the case in which Yc is greater than -Bo/(So-S). This is mathematically due to the requirement that the function f = (Bo+YcSo-YcS)/Bo be greater than zero in order for the logarithm of the function to be real. Physically, this is due to the fact that B cannot in reality be negative. It should be noted that the sensitivity of the variable-biomass models to Yc is dependent on Bo, and vice versa, as the two parameters are interrelated.

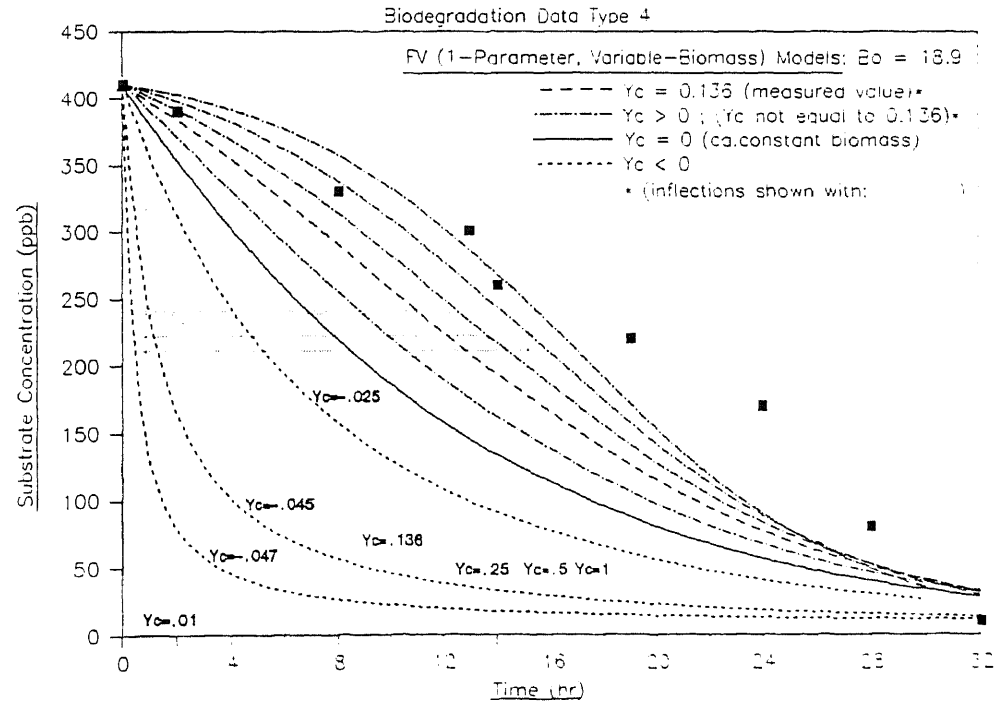
Figure 38 shows FV to be the best of the first-order models evaluated. Unlike F1 and F2, FV exhibits a downward bend with an inflection at t = (1/(ko(Bo+YcSo)))ln(YcSo/Bo) followed by the more conventional first-order curvature. This effect is more readily apparent in Figures 41 and 42 which show the response of the FV curves to changes in Bo and Yc, respectively, for this data set. These figures both show

Figure 41



Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Figure 42

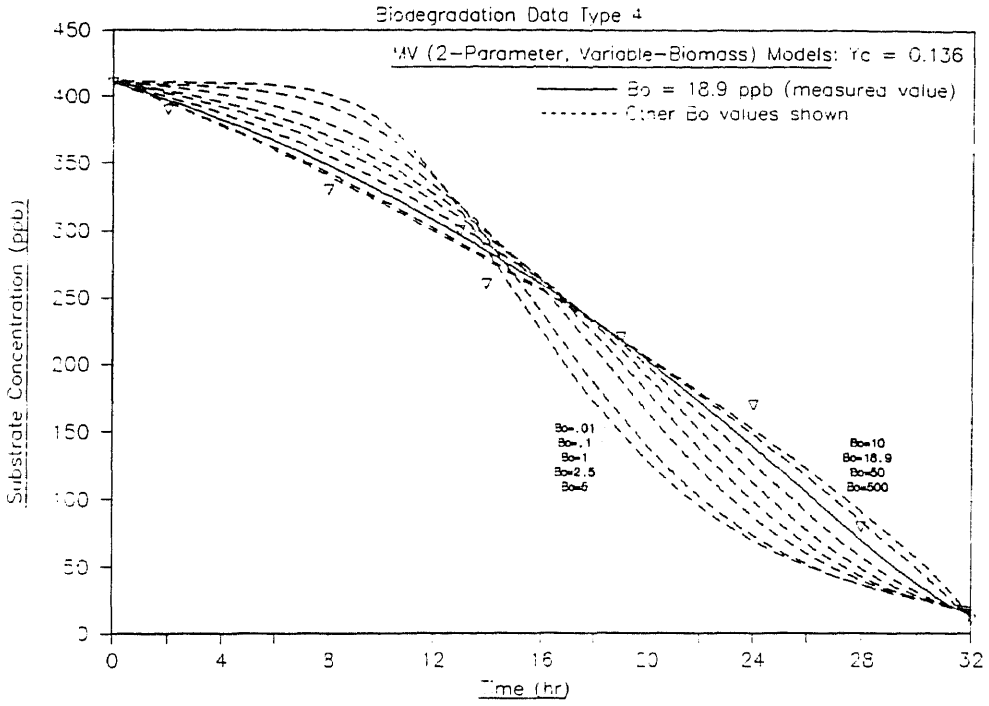


Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

increased variable-biomass effects (i.e., initial biodegradation rate approaches 0 while the ultimate biodegradation rate approaches infinity) as either Bo is decreased or Yc is increased. Conversely, constant-biomass behavior (i.e., the F1 curve) is approached as Bo increases or Yc decreases. The two figures show that, as either Bo increases or Yc decreases, the inflection occurs at correspondingly lower values of t until such a point as it drops below zero and is no longer visually apparent (note: for negative values of Yc, inflections do not exist at all).

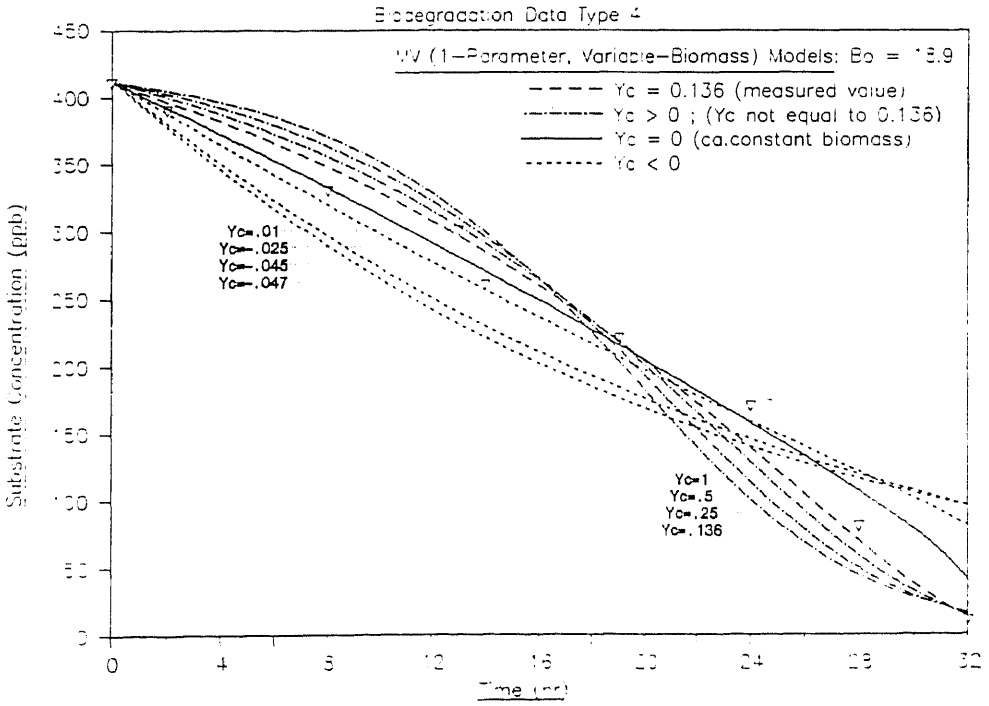
Figure 42 also shows that negative values of Yc result in the prediction by FV of the equivalent of a greater-than-first-order drop. As stated previously for the ZV models, FV curves can be predicted only for negative values of Yc in which Yc is greater than -Bo/(So-S). It is apparent from Figures 41 and 42 that the FV model is especially sensitive to the values of Bo and Yc. Qualitatively, the FV model possesses similar characteristics to the MV model and it may be difficult to classify a data set as either FV or MV based on visual inspection of the data alone. The MV model, however, is visually and statistically much better for type 4 data, and is also much less sensitive to errors in Bo and/or Yc as seen in Figures 43 and 44 which show the corresponding MV curves for the same values of Bo and Yc shown in Figures 41 and 42, respectively. The MV curves have the ability to better model a more gradual transition from initial to maximum biodegradation rate compared to the FV curves. As a side note, Figure 44 shows the MV model

Figure 43



Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

Figure 44



Source : Klecka, G.M. & Maier, W.J. (data set #3 on pages D-45 & D-46)

to lose its inflection and resemble the FV model when negative values of Yc are used (although the effect is less pronounced for the MV model).

While the MV model is less sensitive in terms of fit than the FV model to errors in Bo and Yc, it may result in regression of negative values of K for some data sets if Bo and Yc do not correspond to a sufficient enough variable-biomass effect. For example, the MV model yields negative values for K in Figure 43 when Bo is greater than 35 ppb and in Figure 44 when Yc is less than 0.08. To avoid this problem with the MV model inadequately representing type 4 data, it is crucial that biomass measurements be accurate.

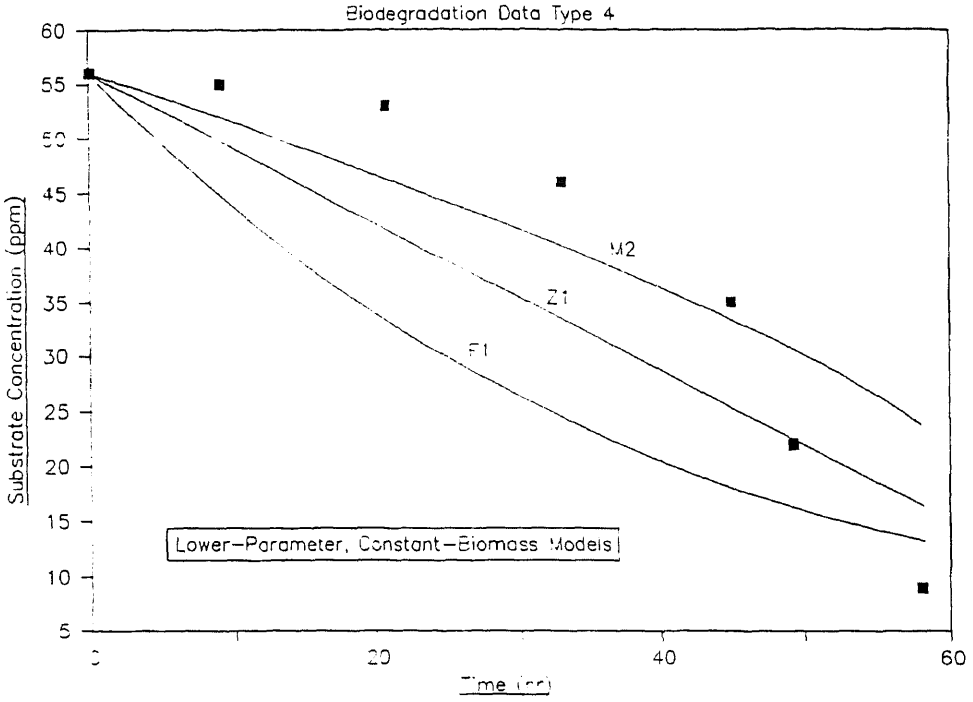
Data set #4 (shown in Figure 35) is analogous in behavior to data set #3 which was discussed extensively above. Data set #4, however, covered a lower S range which, in turn, resulted in a higher relative percentage error in S measurements. This increased uncertainty resulted in reduced confidence in model selection as the statistical differences between the model types are less significant (refer to pages D-47 and D-48). The variable-biomass models still, however, perform better than the constant-biomass models, with MV being the best. Note that the M2 is the only one of the three Monod models to regress a negative value of K for this data set. While the values of Bo and Yc appear reasonably accurate for this case, they are not optimum in that they do not result in the best possible fits for the three variable-biomass models evaluated. Furthermore, the values of Bo and Yc which

yield the best fit for one of the variable-biomass models (e.g., MV) does not necessarily yield the best fit for the others (e.g., FV and ZV).

Papanastasiou and Maier studied the mutual-inhibition effect of a glucose/2,4-D, dual-substrate system of which Figure 45 presents the S vs t curve for one of the two substrates (i.e., 2,4-D). The authors fit their data using a modified Monod equation that incorporated a term to account for inhibition by alternative substrates as described by Yoon, et al.[5] Whereas this model is better than the models evaluated in this thesis for predicting the behavior of this specific dual-substrate system, it may be too complex and specific to be of value as a general purpose tool.

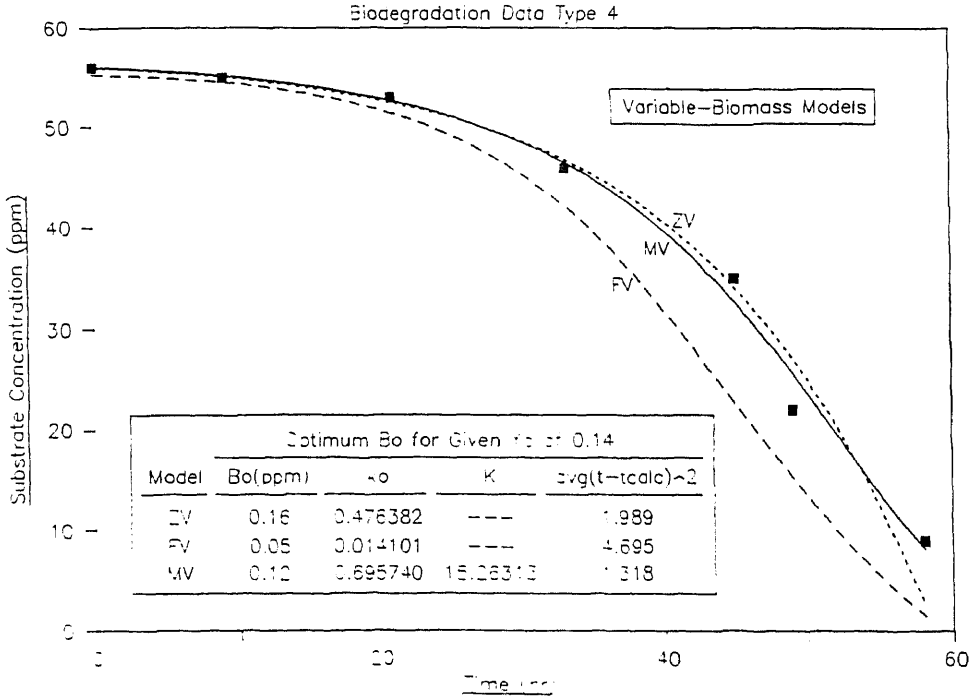
The lower-parameter, constant-biomass models are graphically shown in Figure 45 to be terrible in representing the data set which apparently exhibits a very strong variable-biomass effect. The authors, however, did not provide sufficient biomass data (i.e., Yc was given but Bo was not) to assess the variable-biomass models, and hence, the corresponding tabulation for this set is not given in Appendix D. Figure 46, however, graphically shows the three variable-biomass models (i.e., MV, ZV and FV) for the cases in which Bo was selected (i.e., with Yc being set at the given value) so as to minimize the value of $\Sigma(t-tcalc)^2$. The data set is best represented by the MV model. While the ZV model is reasonable over the range considered, significant errors will result when extrapolating outside the range due to the inability of ZV to represent the inflection and subsequent first-order

Figure 45



Source : Papanastasiou, A.C. & Maier, W.J. (data set #3 shown on page D-57)

Figure 46



Source : Papanastasiou, A.C. & Maier, W.J. (data set #3 shown on page D-57)

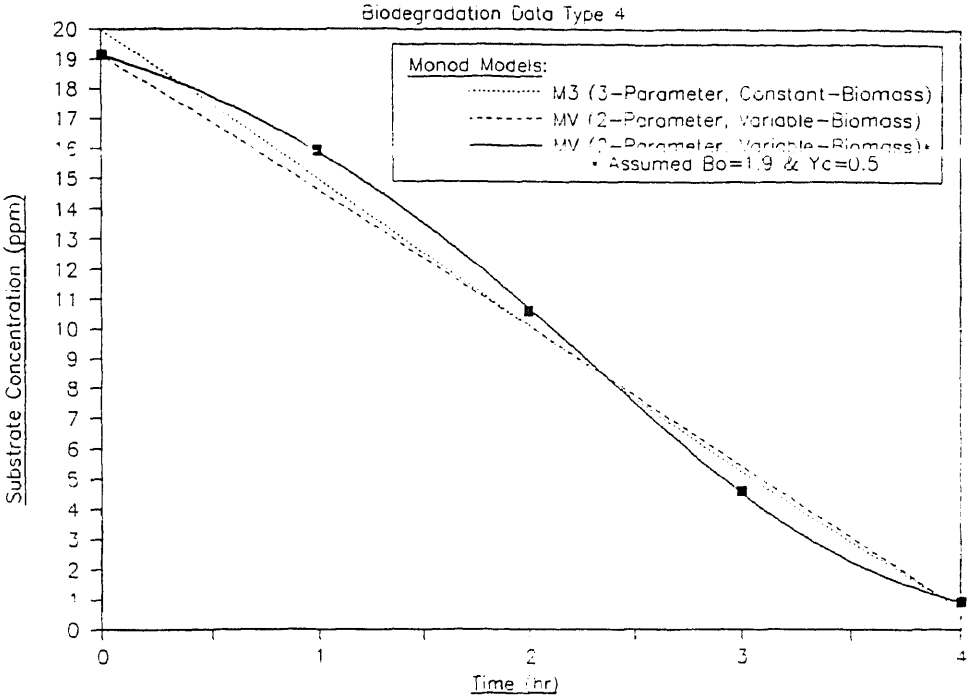
effect. The FV model, while characteristically correct in terms of general curvature, is less flexible than the MV model and has greater difficulty fitting data which are not very nearly first order.

The optimum values of Bo shown in Figure 46 are slightly different for each of the three models. The value for MV is intermediate between those for ZV and FV, which is to be expected since the data is intermediate between zero and first order. In each of the three cases, Bo is very low which is characteristic of such a system with a pronounced variable-biomass effect. It is highly unlikely that the author's measurements would have provided such a low value for Bo since the culture was an activated sludge with an expected total biomass concentration of 1000-5000 ppm. None of the commonly-used, biomass-measurement techniques accurately differentiate active from inactive biomass, especially when the active cells are at such a low level relative to the total population.

It should be noted that the M2 and M3 models both regressed negative values of K for the data set presented in Figures 45 and 46. While the MV model yielded a positive value of K for the case shown in Figure 46, a negative value would be obtained for higher values of Bo where the variable-biomass effect is sufficiently diluted such that the model is forced to regress a negative K in order to fit the predominantly downward bend in the given data set.

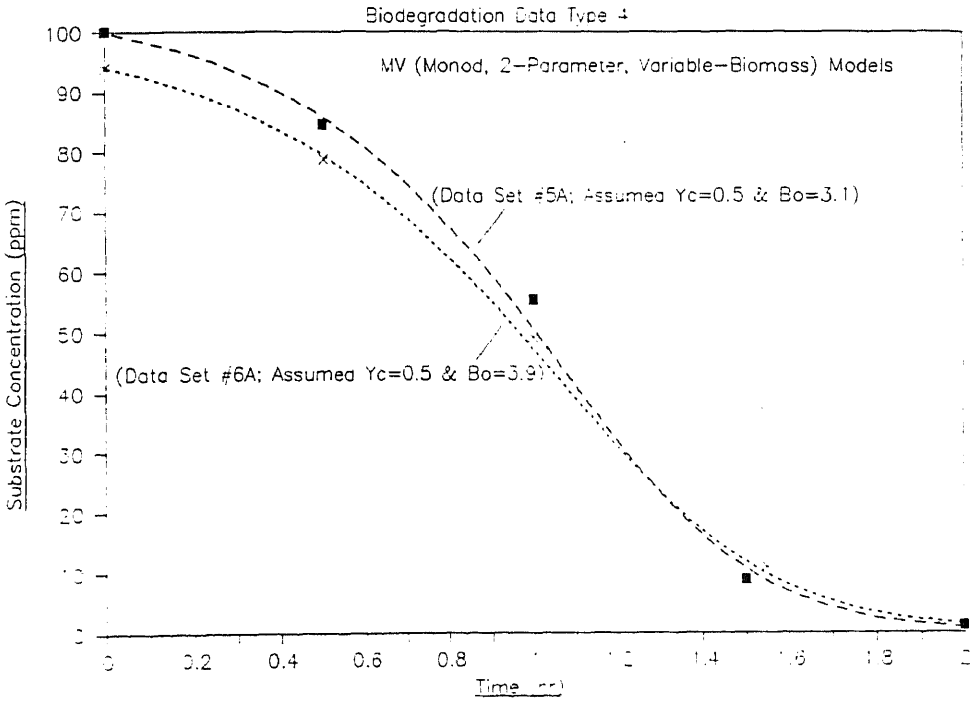
In addition to the 4 data sets discussed thus far in this section, 3 more of the 124 mixed-culture systems evaluated in this thesis were classified as type 4 (refer to Figures 47 and 48). Figure 47 presents the M3 and MV models regressed from the available data shown on pages E-10 and E-11, as well as an MV model for which an optimum value of Bo (i.e., such that $\Sigma(t\text{-}tcalc)^2$ was minimized) was selected for an assumed value of 0.5 for Yc. The former two are notably worse than the latter. The data summaries on pages E-10 and E-11 show the Monod models in general to be little better than the zero-order models. M2 and MV, in particular, yield negative values of K, while only M3 regresses a positive value. The optimum MV curve shown in Figure 47 also yielded a positive value of K. The reason for the poor performance of the MV model shown on page E-11 is the inaccurate biomass measurements which resulted, for one thing, in an unrealistically high value of Yc. Of more importance than the Yc value is the fact that the Bo value is a measure of the total biomass concentration and <u>not</u> the viable biomass level. As a result, the Bo value is excessively high accounting for the predicted variable-biomass effect being much less than that observed. For example, the predicted increase in biomass concentration is only 8.9% for the case shown on page E-11 versus 480% for the optimum fit shown on Figure 47.

Figure 47



Source : Colish Thesis (data set #3 shown on pages E-10 & E-11)

Figure 48



Source : Naik Thesis (data sets #5A & #6A on pages E-70 & E-73, respectively)

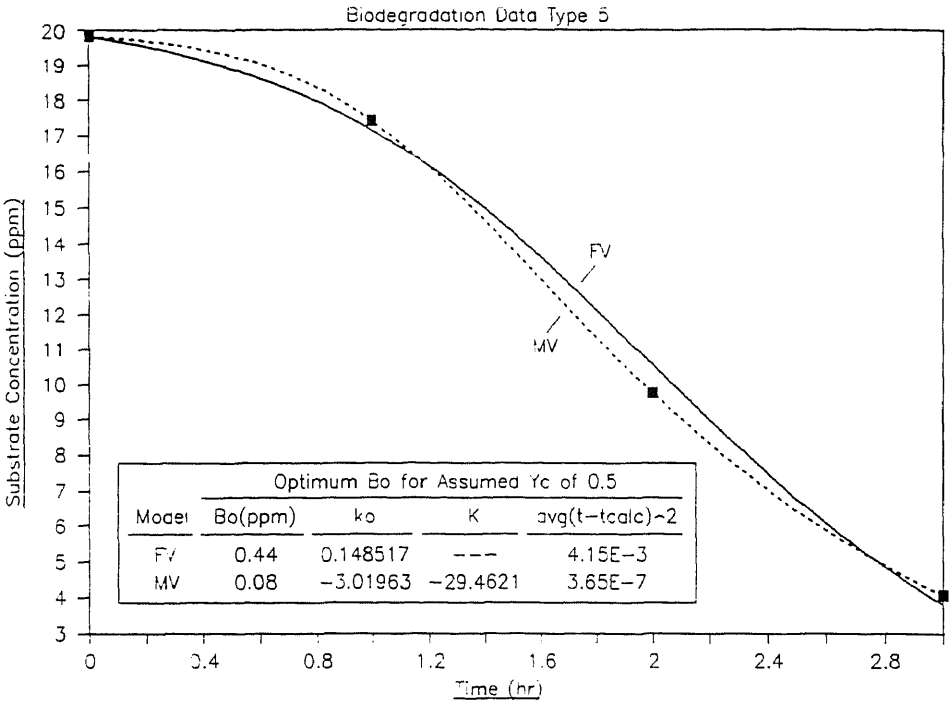
Figure 48 presents two data sets from the Naik thesis for the same system with the optimum MV curves shown. The variable-biomass models were not evaluated utilizing actual biomass measurements because of the inherent nature of the multiple substrate system involved which made determination of the substrate-specific parameters of Bo and Yc impractical.

6.1.5 Date Type 5 (First-Order, Variable Biomass)

This biodegradation data type can be considered a limiting case of data type 4 in which S is kinetically limiting relative to B. This data type is well represented by the FV model with Figures 41 and 42 in Section 6.1.4 visually presenting the characteristic features of this data type as well as the effect of the parameters Bo and Yc on the regressed FV curves.

Figure 49 shows the data set from pages E-12 and E-13 to be reasonably well represented by a hypothetical FV model (i.e., Yc assumed to be 0.5 and Bo was then selected so as to minimize $\Sigma(t\text{-}tcalc)^2$). The performance of this FV model is significantly better than the models on pages E-12 and E-13. The M2 and M3 models regress negative values of K to fit the predominantly downward bend in the data while the MV model does the same because of the inherent inaccuracy of the measured biomass data (i.e., "total", not "viable", biomass was measured) which results in an underprediction of the observed variable-biomass effect (e.g., the measured biomass increased by only 5.2% over the range of S consumed while the optimum FV curve predicts an 1800% increase in order to model the observed effect).

Figure 49



Source : Colish Thesis (data set #4) ; refer to pages E-12 & 13

Figure 50

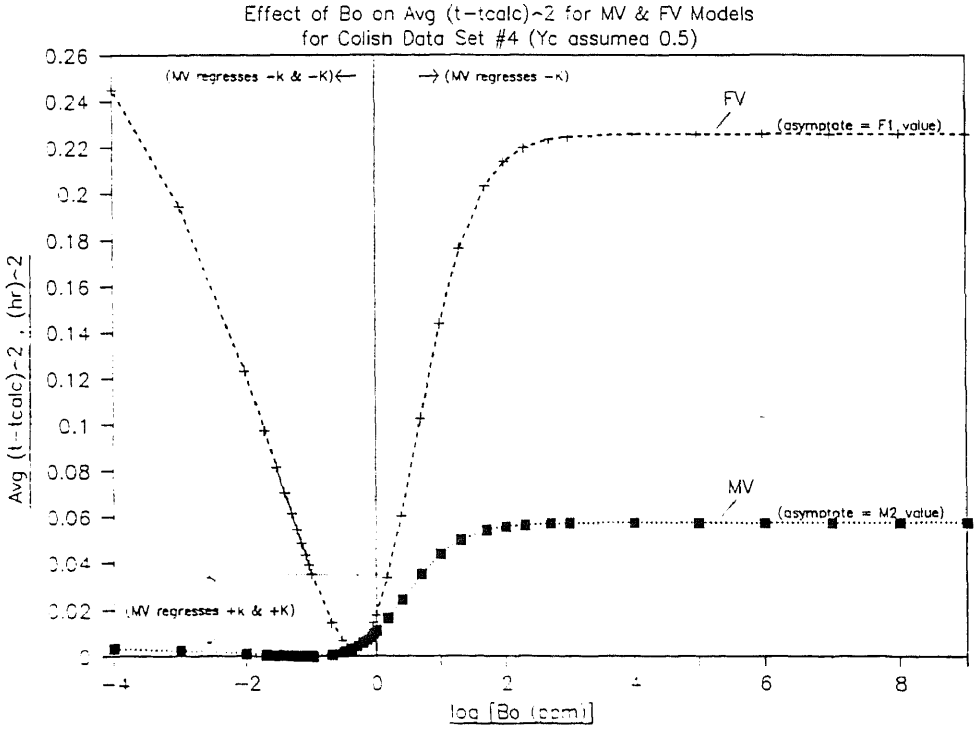


Figure 49, in addition to the hypothetical FV model, shows a hypothetical MV model to fit the data perfectly. The MV model, however, regresses negative values of both k and K because of the data being interpreted by the model as greater than first order for the values of Bo and Yc used. Figure 50 graphically presents the effect of Bo on the fit of the data (shown in Figure 49) in terms of the statistic $\Sigma(t\text{-}tcalc)^2$ for both the FV and MV models. This plot again demonstrates the point made previously in Section 6.1.4 that the FV model is much more sensitive to errors in biomass measurements than MV. The MV model, however, is also extremely sensitive to inaccurate biomass measurements from the perspective that negative kinetic parameters may be regressed (refer to Figure 50 to see the relatively small range of Bo values for which MV regresses positive values of both k and K). The data set in Figure 49 is classified as FV and not MV because the optimum FV curve results in a lower $\Sigma(t\text{-}tcalc)^2$ than the optimal MV for which positive kinetic parameters are obtained. The MV model will always result in a better fit of type 5 data than the FV because of the additional degree of freedom provided by the kinetic parameter K in the former. Because type 5 data will always possess some experimental error, however, the MV model has an approximately equal probability of regressing either both positive (if the data is interpreted by MV as being less than or equal to first order) or both negative values (if the data is interpreted by MV as being greater than first order) for k and K,

provided the biomass data are accurate. As a result of this, the FV model is preferred over the MV for type 5 data.

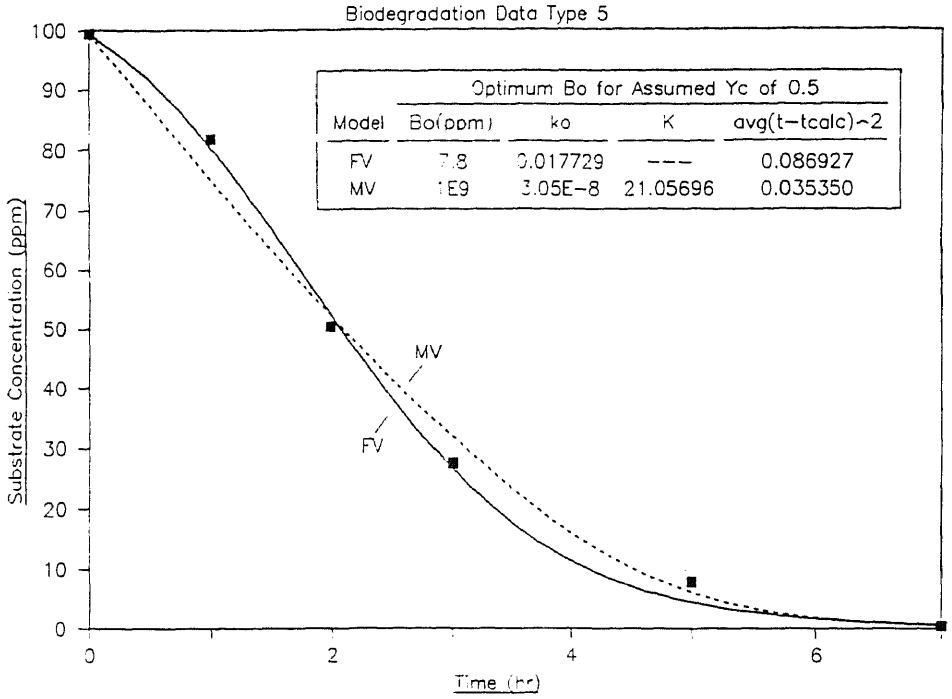
Figures 51 and 52 present two more examples of type 5 data with the optimal MV and FV curves shown in each case. In both cases the Monod model is statistically slightly better. In Figure 51, MV yields positive rate constants while in Figure 52 it yields negative rate constants. Figure 51 shows the optimal MV curve to be that for the limiting case of constant biomass.

6.1.6 Data Type 6 (Zero-Order, Variable Biomass)

This biodegradation data type is a limiting case of type 4 data where B is kinetically limiting relative to S (i.e., S>>B) over the entire range of S covered . These autocatalytic reactions are terminated before the biodegradation rates reach their maximum value (i.e., no inflection is obtained). This data type is well represented by the ZV model with Figures 39 and 40 in Section 6.1.4 visually presenting the characteristic features of this data type as well as the effect of the parameters Bo and Yc on the regressed ZV curves.

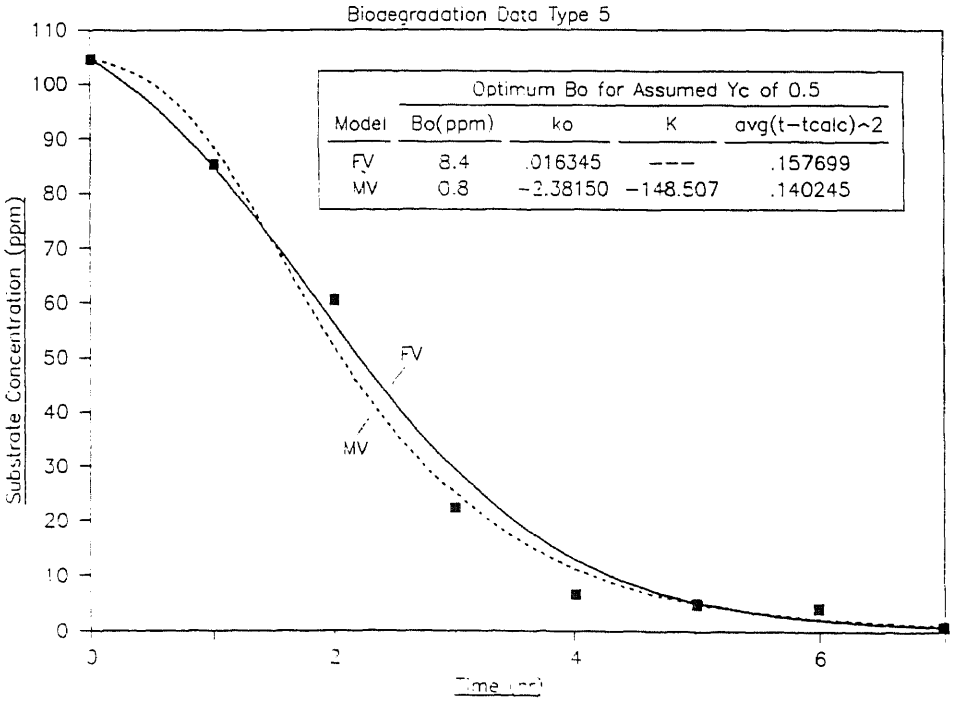
As mentioned previously in Section 6.1.1, most industrial problems involve removal of pollutants down to very low levels where S is limiting relative to B and first-order curvature is apparent. Operation under substrate-limiting conditions is also desired in activated-sludge, wastewater treatment facilities so as to minimize bacterial growth (i.e., via endogenous respiration) since disposal of excess sludge is both

Figure 51



Source : Naik Thesis (data set #4A) ; refer to page E-67

Figure 52



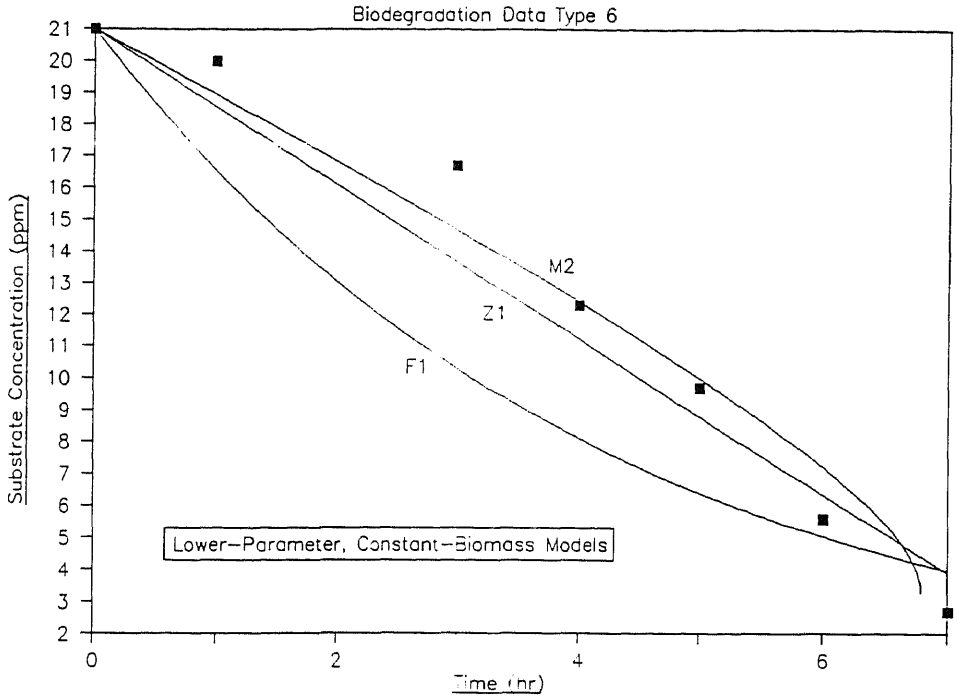
Source : Pak Thesis (data set #10) ; refer to page E-106

problematic and costly. It is, therefore, natural that most laboratory studies would logically operate under similar conditions. This is exactly what was observed in the cases studied in this thesis as only 2 of the 116 mixed-culture systems were categorized as type 6 data.

Figure 53 presents the first of the two data sets categorized here as type 6, along with the corresponding lower-parameter, constant-biomass models from page E-39. None of the constant-biomass models are appropriate for data of this sort. Z1 and Z2 cannot model any curvature, while F1 and F2 predict curvature opposite to that actually observed. Whereas M2 and M3 can model the downward bend inherent in data of this type, they do so via the regression of negative values of K and are, therefore, not valid.

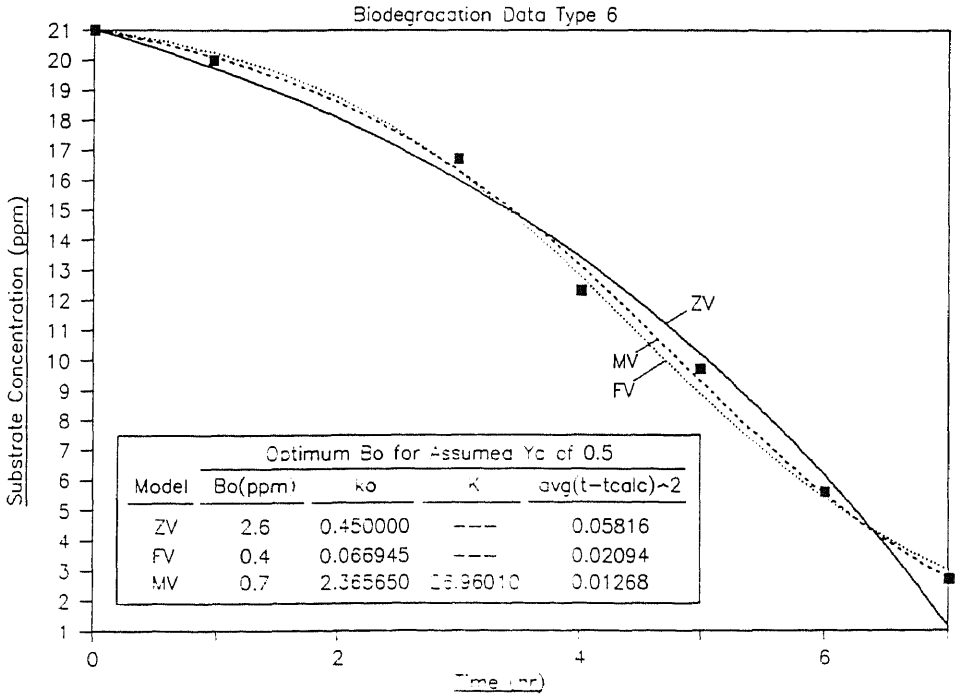
Figure 54 shows the same data set to be well-fitted by all three variable-biomass models. Each of the three curves are hypothetical and represent the best possible fit for each model type for the case in which Yc is assumed to have a value of 0.5. Because of the scatter in the data and the lack of information as to the magnitude of the experimental error, it is not possible to select one (with any high degree of confidence) as being the "correct" depiction of reality. While the Monod is statistically best (as always), its regression is sensitive to the accuracy of biomass measurements with respect to obtaining

Figure 53



Source : Gonnabathula Thesis (data set #10B) ; refer to page E-39

Figure 54

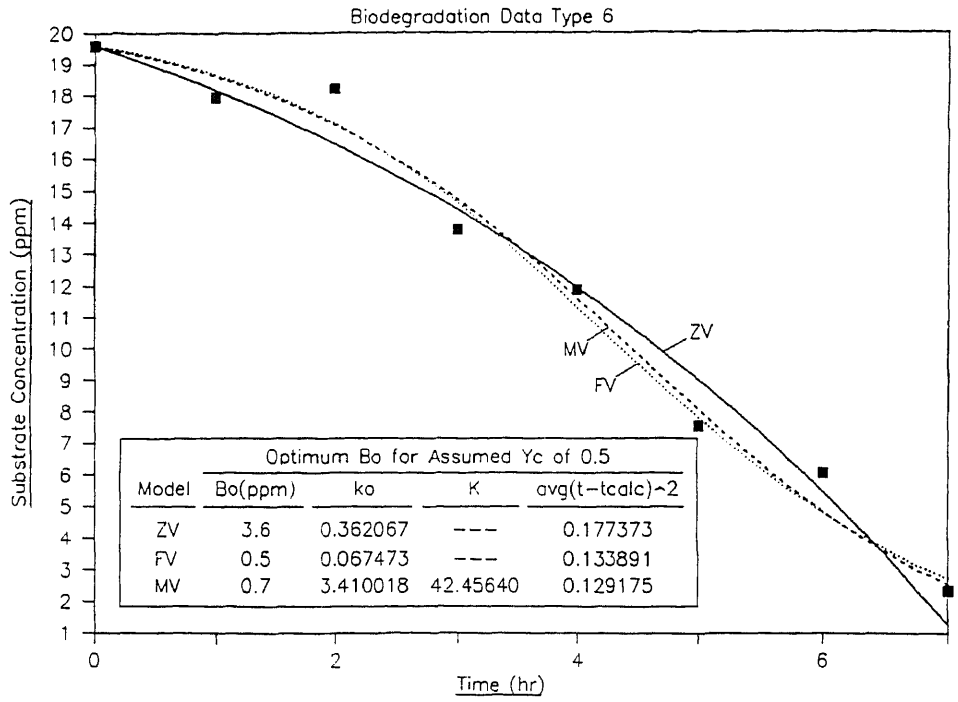


Source : Gonnabathula Thesis (data set #10B) ; refer to page E-39

positive rate constants (as mentioned previously in Sections 6.1.4 and 6.1.5); negative values of K are obtained in this case for values of Bo > 4 ppm and negative values of both k and K are obtained for values of Bo $\leq$ 0.3 ppm. Furthermore, while MV provides a statistically better fit than ZV, it may be overfitting the experimental error in the data and not necessarily better representing reality. For both of these reasons, the ZV model is generally preferred over the MV for type 6 data, but only over the range of S and conditions covered (i.e., ZV is not appropriate for extrapolation because of an imminent transition to first-order kinetics). The FV model happens to fit this data set nearly as well as the MV. As mentioned previously (refer to Figure 50), however, the FV model is extremely sensitive to the accuracy of biomass measurements. For values of Bo not immediately near the optimum, the FV model becomes significantly worse than the ZV.

Figure 55 presents the only other data set categorized as type 6. None of the constant- or variable-biomass models regressed on pages E-8 and E-9 are very good representations of the system. While the constant-biomass models suffer for the same reasons as stated on page 90 for the data set shown in Figure 53, the variable-biomass models suffer from inaccurate biomass measurements. Colish measured bulk biomass and not the active bacterial population. The substrate used (i.e., o-chlorophenol) is relatively resistant to biodegradation and, as such, only a small percentage of the overall sludge would be expected to be able to utilize it.

Figure 55



Source : Colish Thesis (data set #2) ; refer to pages E−8 & E−9

Figure 56

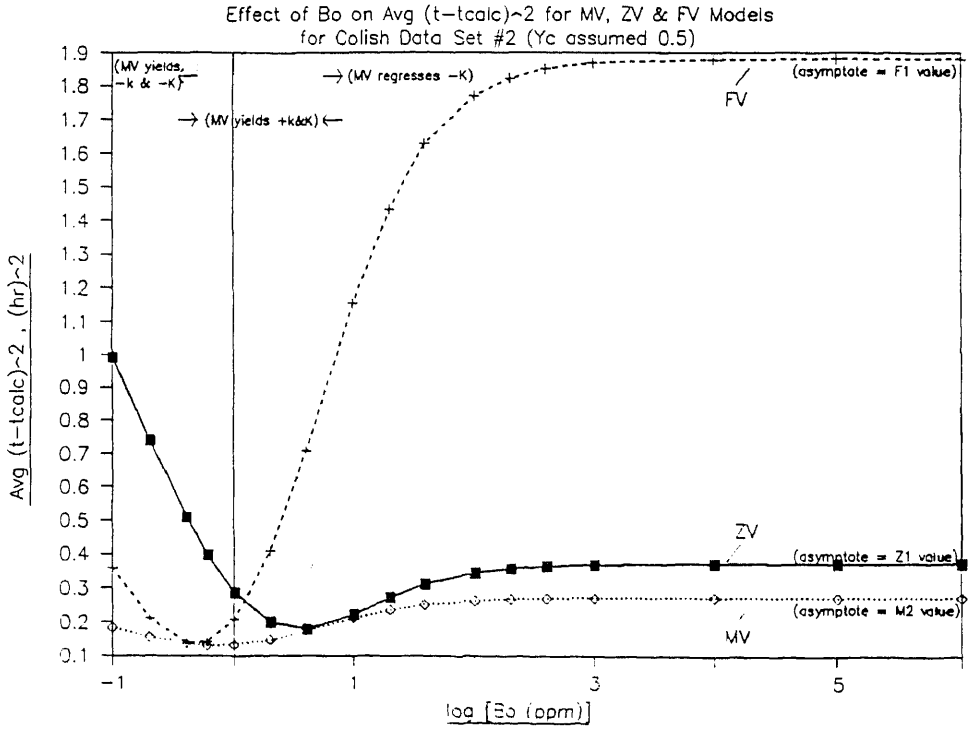


Figure 56 shows the effect of Bo on the fit of the three variable-biomass models to the data set presented in Figure 55 for an assumed Yc value of 0.5. While the Monod is statistically best over the entire range, it requires accurate, viable-biomass measurements in order to regress positive coefficients. FV also requires accurate, viable-biomass measurements in order to obtain a good fit. ZV is less sensitive to errors in Bo and is only slightly worse than MV over the practical range of interest and is, therefore, preferred for type 6 data. Figure 55 graphically presents the optimum fit for each of the three variable-biomass models from Figure 56 (i.e., for the value of Bo which minimizes $\Sigma(t\text{-}tcalc)^2$). All are feasible for the data set presented. Selection of the "true" model for this data set is hindered by the data scatter and lack of information from the author as to the magnitude of the experimental error.

6.1.7 Data Type 7 (Lag followed by Biodegradation)

Biodegradation data type 7 consists of the broad group of S vs. t curves where lags are apparent. The portions of the curves following the lags may be characteristic of any of the first six biodegradation types discussed thus far. The lag represents the acclimatization of micro-organisms to a substrate. During the lag, the bacterial cells have long generation times and are characterized by zero growth rates. Nutrients are taken into the cells and the mass of bacteria increases as the amount of enzymes and nucleic acid increases. Once a

sufficient amount of the substrate-specific enzymes are generated, biodegradation takes place as discussed in the previous sections. The length of the lag period is variable (i.e., it is dependent on the size and degree of adaptation of an inoculum to its new environment). Lags are common in batch-reactor studies where the sludges are not sufficiently acclimated to the substrates.

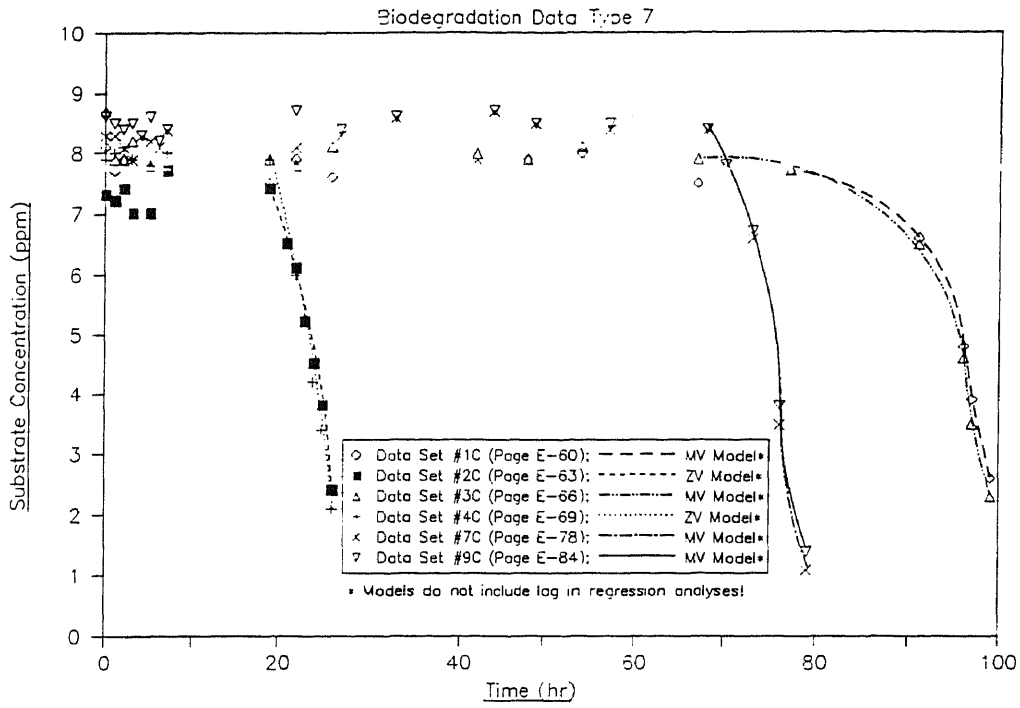
None of the models evaluated in this thesis are theoretically capable of depicting the often abrupt transition from lag to utilization characteristic of this data type. The ability of the models studied herein to reasonably well fit data sets of this type is largely dependent on the length of the lag relative to the overall biodegradation time (e.g., the shorter the lag, the better the potential fit). For the case of the constant-biomass models, the higher-parameter versions are notably better than the corresponding lower-parameter versions because of their ability to average the error, in the initial portion of the S vs t data, resulting from the models' inherent inabilities to properly fit the lag. The variable-biomass models are potentially better (depending, in part, on the accuracy of Bo and Yc) than the constant-biomass models for data of this type, but their dependency on accurate biomass measurements limits their practical usefulness. The best approach for data of this type is to disregard the lag and fit the remaining biodegradation portion of the S vs t data. The appendices, however, present the results for each complete data set as

given by the corresponding sources; the segregation approach (i.e., separation of the lag from the data set before performing the kinetic analysis) is demonstrated graphically within this section for comparative purposes only. As stressed previously, it is imperative that the system (i.e., biomass composition/concentration, etc.) be well-defined in order for the kinetic analyses to be useful for design purposes.

The lag measured on laboratory scale in batch reactors is often not regarded as a concern in large-scale facilities, which consist of continuous reactors operating under the assumption of steady state. Knowledge of the activity of the acclimated sludge for a specific substrate (which is typically derived from batch reactor studies), however, is crucial to the design and performance of these continuous units. Furthermore, the assumption of steady state is not always valid, as the feedstock to wastewater-treatment facilities may vary significantly and, as such, specific information on the unsteady-state behavior of a sludge in response to these changes is necessary to ensure proper operation.

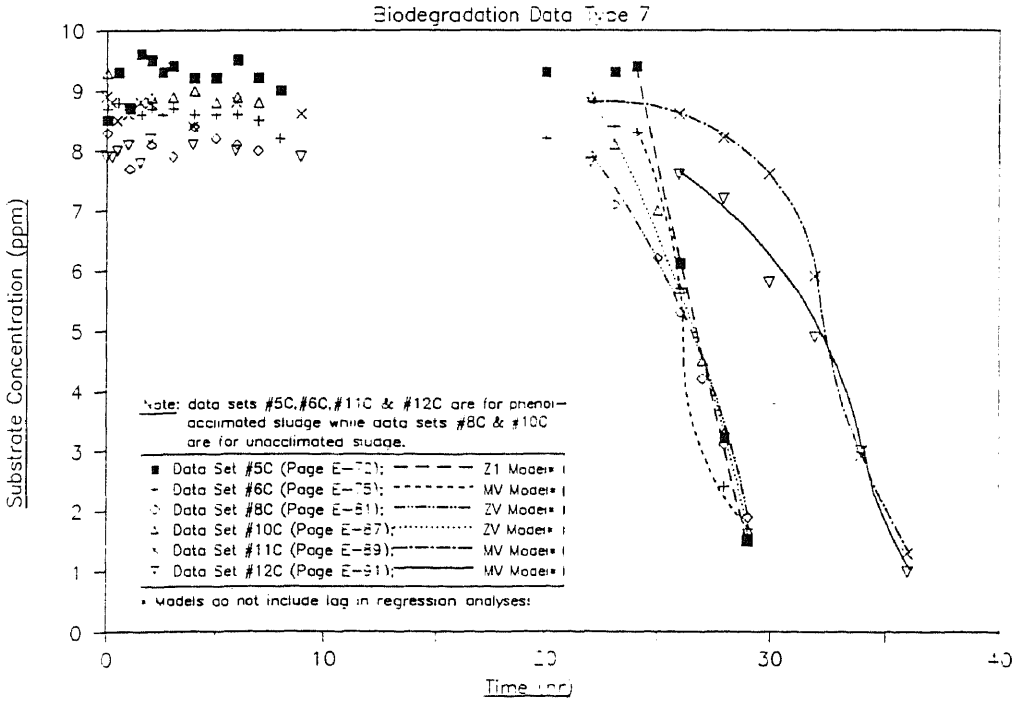
The commonality of the occurrence of lags in batch-reactor studies is apparent in this thesis as 44 of the 124 data sets reviewed (for mixed-culture systems) possess them. Figures 57 through 66 show all 44 of the data sets along with the models best deemed to represent them.

Figure 57



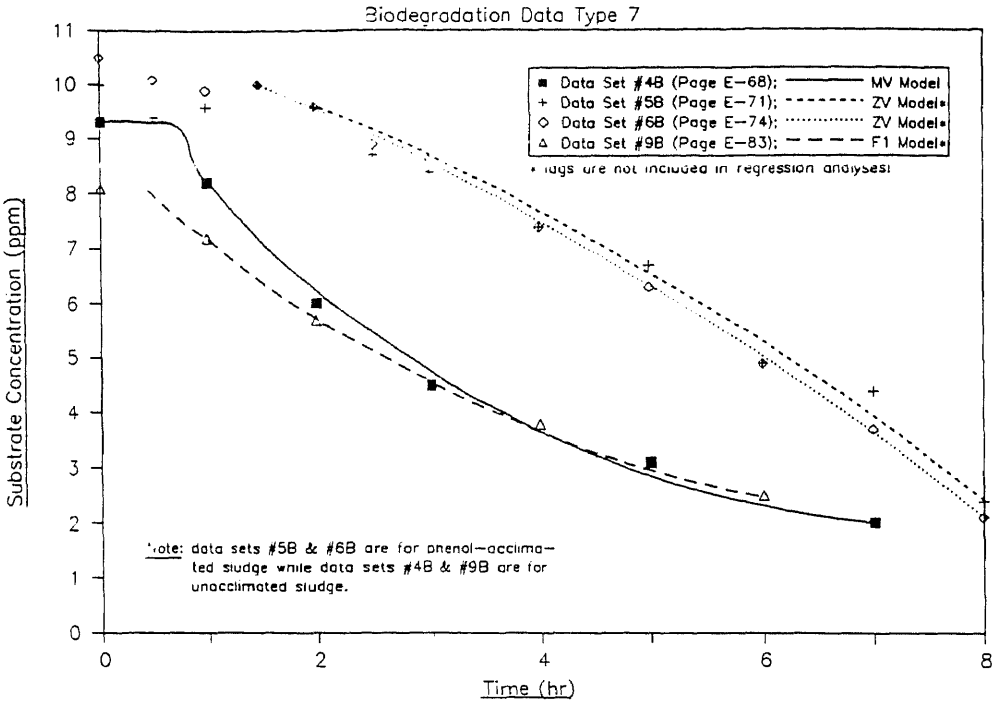
Source : Naik Thesis (2,6-dichlorophenol in unacclimated sludge)

Figure 58



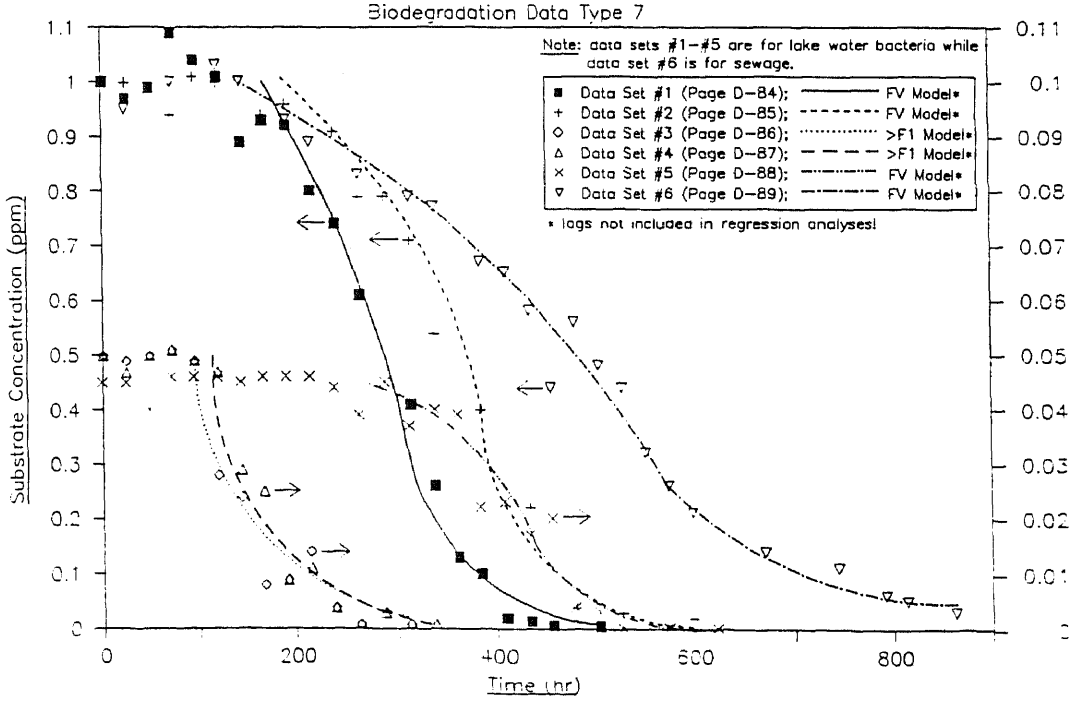
Source : Naik Thesis (2,6-dichlorophenol as substrate)

Figure 59



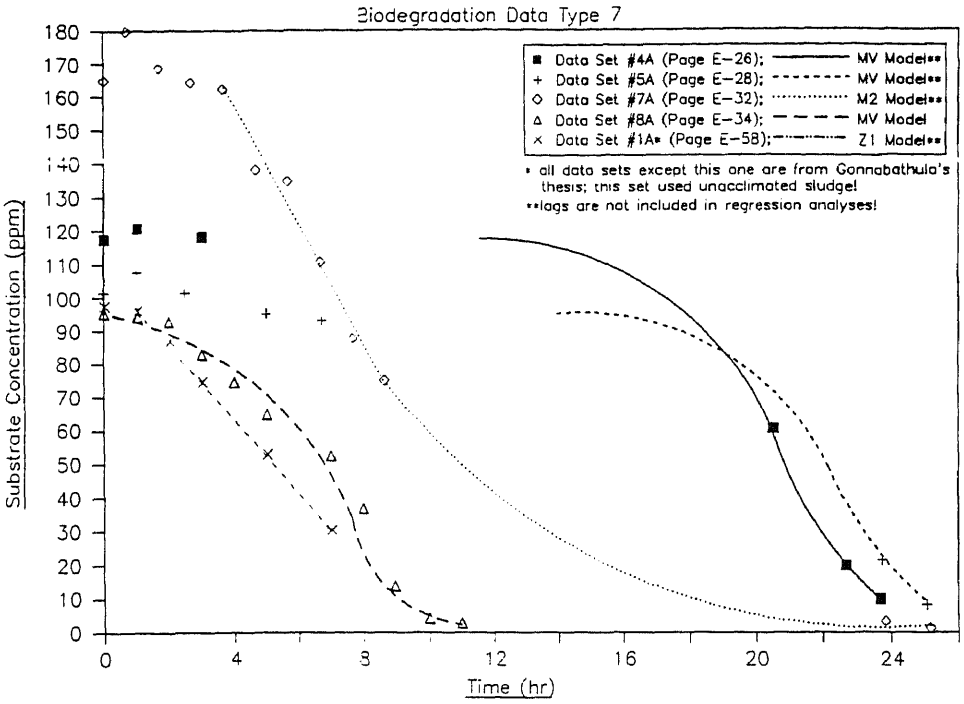
Source : Naik Thesis (nitrobenzene substrate)

Figure 60



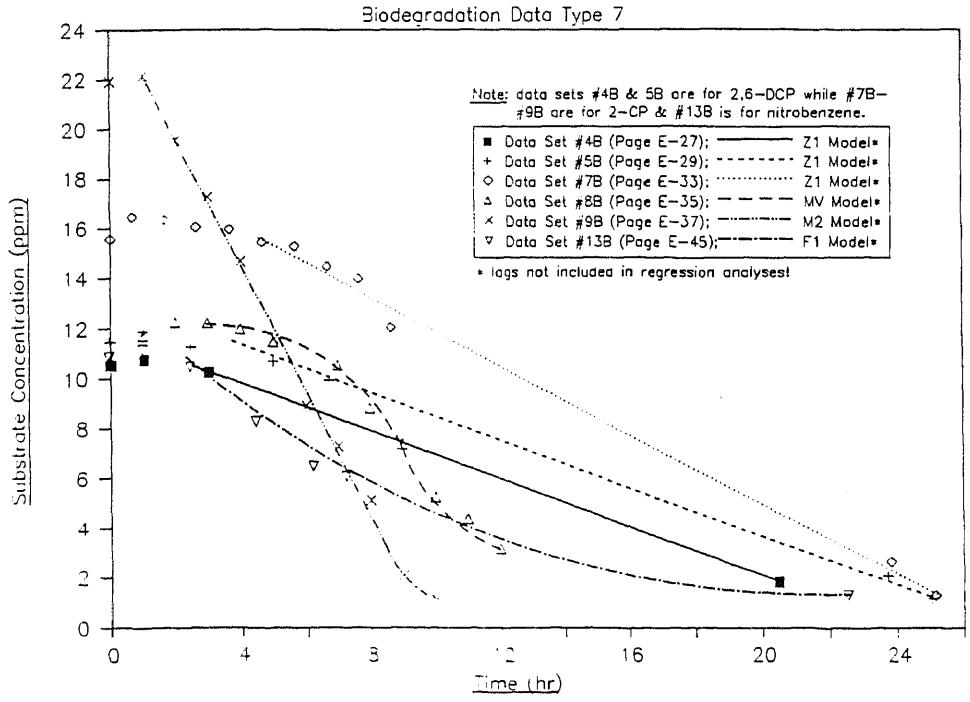
Source : Yoray, J.R. & Alexander, M. (N-nitrosodiethanolamine as substrate)

Figure 61



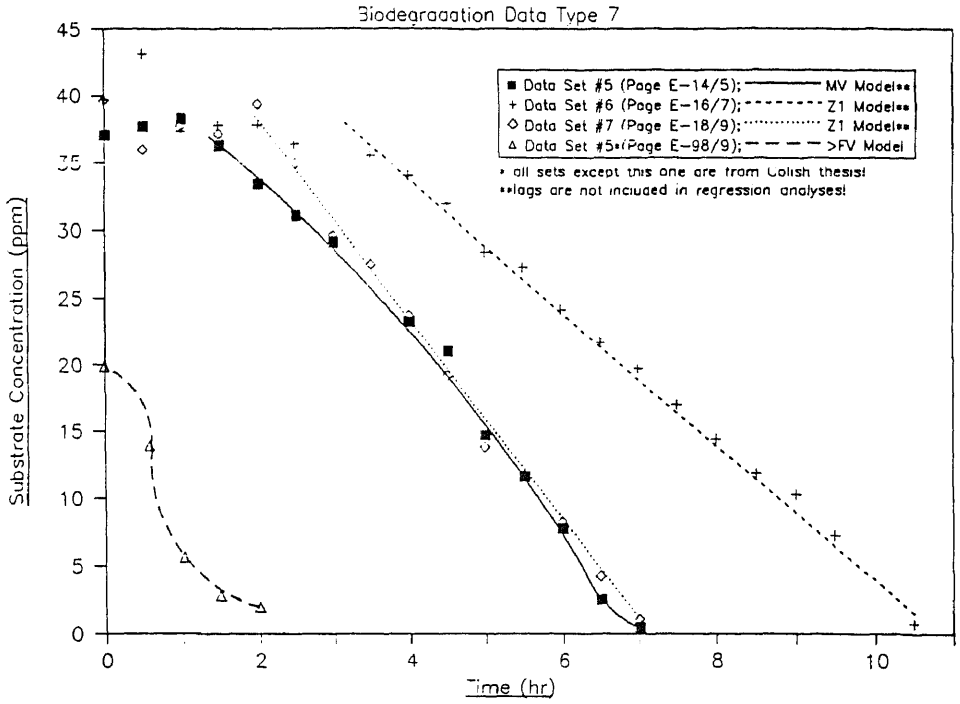
Source : Gonnabathula & Naik Theses (phenol as substrate in mlss)

Figure 62



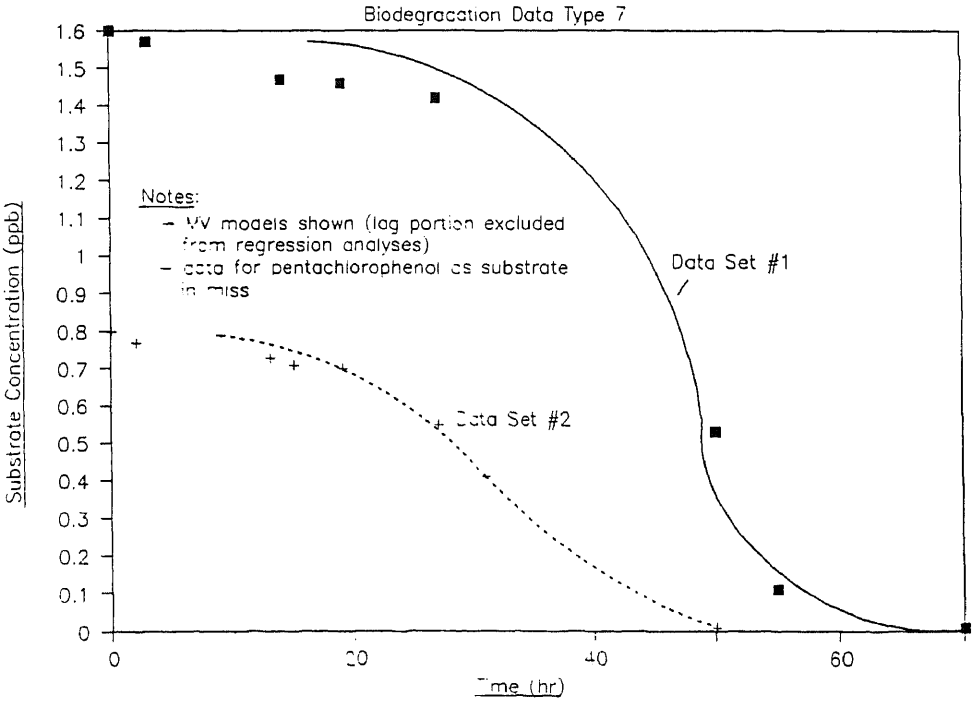
Source : Gonnabathula Thesis (aromatic substrates in mlss)

Figure 63



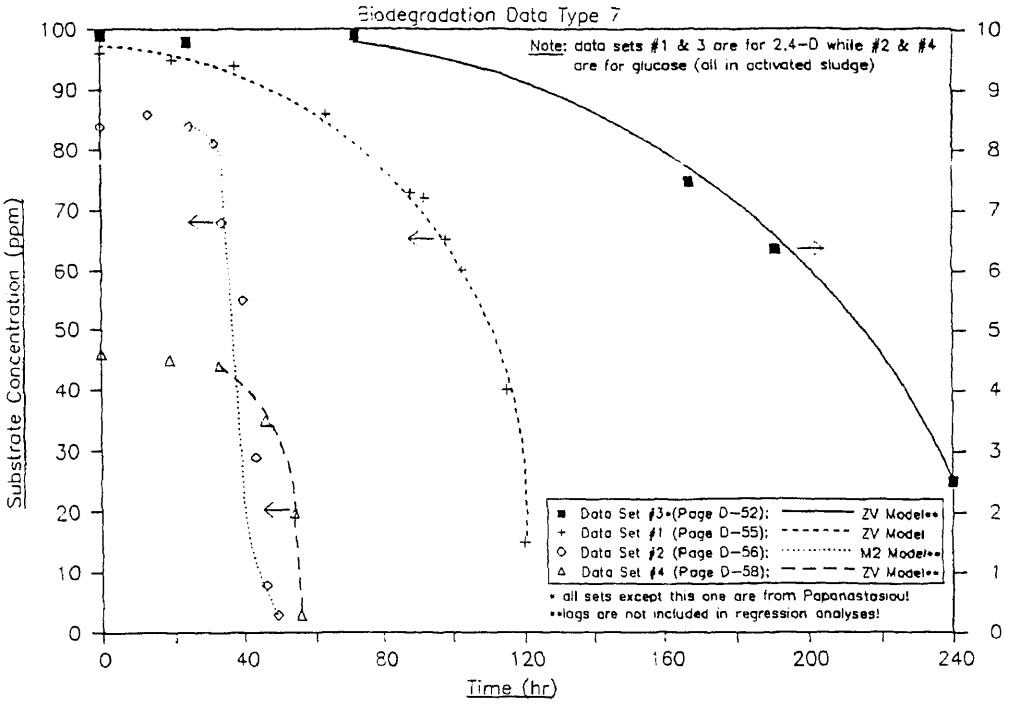
Source : Colisn & Pak Theses (2-chlorophenol as substrate in miss)

Figure 64



Source : Pflecka, G.M. & Maier, W.J. Data sets #1 & #2 on pages D-41 thru 44)

Figure 65



Source : Papanastasiou, A.C., et al and Liu, D., et al.

Figure 66

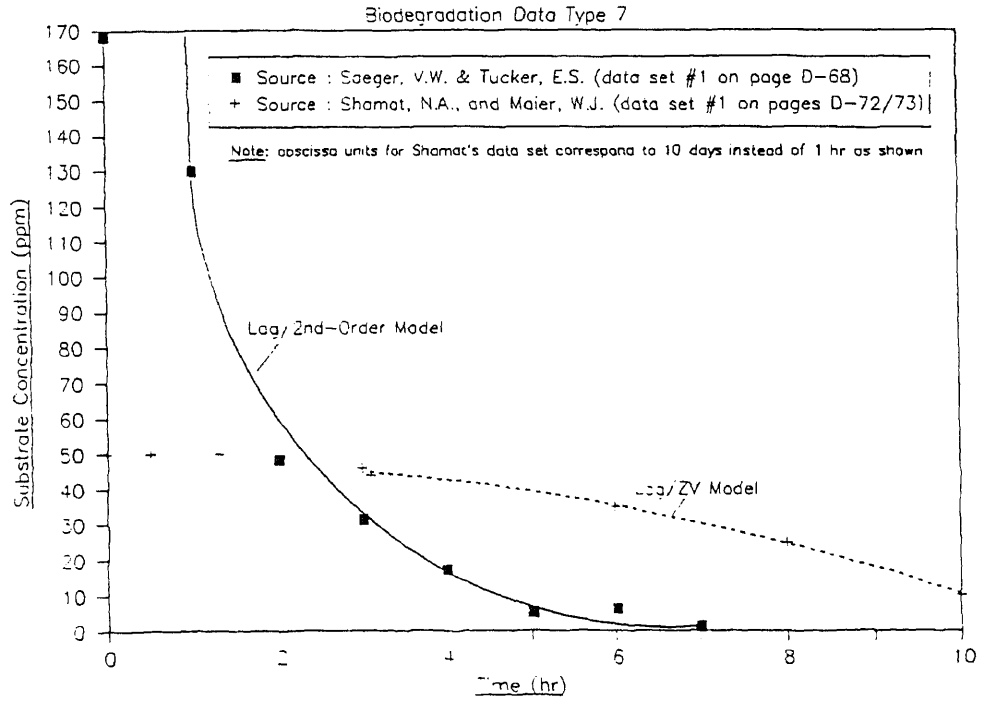


Figure 57 shows six data sets for the same system (i.e., 2,6-dichlorophenol in unacclimated sludge) to yield widely different results in terms of lag length and model type. The differences are attributed to subtle differences between the systems which were not adequately defined by the experiments. For example, "unacclimated" sludges used in data sets #1C and #3C were then used (after partial acclimation in those runs) in data sets #2C and #4C, respectively; even though the sludges had partially acclimated, their classification as "unacclimated" sludge had not changed even though the performance characteristics of the sludges apparently had. The reproducibility between data sets #1C and #3C, and between data sets #2C and #4C (which were both virtually duplicate runs), was excellent. Data sets #7C and #8C were also replicate runs but involved a different co-substrate from the other four runs, thereby accounting for the observed difference in results.

In all six data sets shown in Figure 57, the length of the lags are too long relative to the biodegradation portions to allow adequate representation of the complete data sets by any of the models studied in this thesis. The constant-biomass models are worse than for biodegradation data type 4 (refer to Figure 45 in Section 6.1.4). In all cases, M2 and M3 regress negative values of K to try to fit the downward bend in the data. The zero-order models are unable to model the bend in the data while the first-order models predict curvature opposite to that observed. The variable-biomass models are also unable to adequately

represent the precipitous transition from lag to utilization observed in these sets. As such, the data could only be suitably fitted by models studied in this thesis when the lags were neglected.

Figure 58 presents six more data sets for the same substrate as shown in Figure 57. While the same general comments apply in Figure 58, data set #5C is anomalous in that M2 on page E-72 regresses negative values for both k and K--not just the latter. While it was stated in Section 6.1.2 that this happens when the data apparently drop at a greater-than-first-order rate, it also occurs if the overall trend in the data can be interpreted as S increasing with time (it is noted that S in reality cannot increase with time and that the observed trend is the result of random errors in the measurement of S during a period when biodegradation is not taking place). Because of the restriction of So equal to S(t=0) and because of the bulk of the data being in the lag phase where most of the S values are greater than S(t=0), M2 regresses negative values of k and K to fit the observed data. Figure 17 graphically shows the predicted S vs t curve for a data set in which M3 regressed negative values of both k and K to fit an apparent greater-than-first-order drop. Figure 17 shows that two potential S vs t curves exist for positive values of t. It is the upper portion of the curve which accounts for the minimization of $\Sigma(t\text{-}tcalc)^2$ by the M2 model on page E-72 to result in negative values of k and K. Relaxation of the restriction of So equal to S(t=0) by the M3 model allows it to regress a positive value of k (but not K because of the apparent downward bend in the data set) in this case because of its interpretation of S in the data set as decreasing with time at less than a first-order rate.

Figure 59 shows four data sets (for nitrobenzene as substrate) which have a significantly shorter lag relative to the overall biodegradation time. As a result, the models evaluated in this thesis are better able to approximate complete data sets. Data sets #4B and #9B can be reasonably well-represented by F2 which just averages the error in the lag. M2 and M3 yield negative values of k and K for #4B, unlike positive values for #9B, because of the drop in #4B being greater-than-first-order. MV can (with accurate values of Bo and Yc) fit the data in #4B very well, but it also yields negative values of k and K for the same reason as M2 and M3. It is apparent from data sets #4B and #9B that a lack of data in the initial portions of the curves makes it difficult to be sure whether lags, or variable-biomass effects, or just random scatter in the data points are present. It is, therefore, imperative that biodegradation studies in batch reactors involve sampling at frequent enough intervals, and involve analyses of sufficient enough accuracy, to clearly define the initial lag region, and the transition from lag to utilization.

Figure 60 presents six data sets for N-nitrosodiethanol-amine substrate as measured by Yordy and Alexander. The authors' sole premise was to assess the biodegradability of the specific substrate in various environments. They did not report analytical accuracy nor biomass measurements, nor did they perform any kinetic analyses. The very limited information as to the definition of the system makes the data of little practical value for design purposes.

Figures 61-63 present 15 data sets from three different sources yielding diverse results. Data set #8B in Figure 62 presents another example of M2 yielding negative values of both k and K for data which is not dropping at a greater-than-first-order rate (data set #5C in Figure 58 is the other example).

Figures 64-66 present 8 data sets from a total of 5 different literature sources. Figure 64 shows two data sets for the same system as shown in Figure 35 (refer to section 6.1.4). The length of the lag for this system is observed to increase with So, accounting for Klecka and Maier using the Haldane (substrate-inhibition) form of the Monod expression to model this entire system. Figure 65 presents three data sets from Papanastasiou and Maier which exhibit longer lags than another set from the same study which was previously discussed in Section 6.1.4 (refer to Figure 45). Papanastasiou and Maier used Andrews (substrate-inhibition) model to fit the data for 2,4-D and the MV model for glucose. For the case of glucose, MV can only provide a reasonable fit if the lag is neglected. The authors did not report Yc and Bo for the glucose sets and, hence, comparison with their regressed results could not be facilitated.

Figure 65 also presents a data set from Liu, et al. The authors eliminated abiotic effects from the data via the use of a control, and determined a first-order rate constant (using least-squares analysis) after omitting those points in the acclimation phase. Data set #3 in Figure 65, however, is clearly seen to be of biodegradation type 6 (i.e., ZV) upon excluding the lag portion; the first-order model assumed by Liu, et al, is totally inappropriate for this set.

Figure 66 shows the last two data sets of type 7. The model shown for the data set from Saeger and Tucker is a second-order model (with the lag excluded). The lack of points in the initial region, combined with apparent scatter in the data, makes it difficult to be sure whether a lag truly exists. While the authors corrected the data for the abiotic substrate-removal mechanisms of chemical oxidation and volatilization, their control involved a sterile environment which did not assess whether adsorption onto biomass was significant. The greater-than-first-order drop observed may be due to the combined effects of adsorption and biodegradation.

The data set in Figure 66 from Shamat and Maier is best represented by the ZV model (with the lag excluded). The authors regressed the data (with the lag portion excluded) to the MV model to yield a μm of 0.05 day^{-1} and a K of 25.3 ppm. The regressed results for the MV model on page D-73 are in reasonable agreement (i.e., $\mu m = ko/Yc = 0.04\ day^{-1}$ and K = 20.6 ppm) considering the following

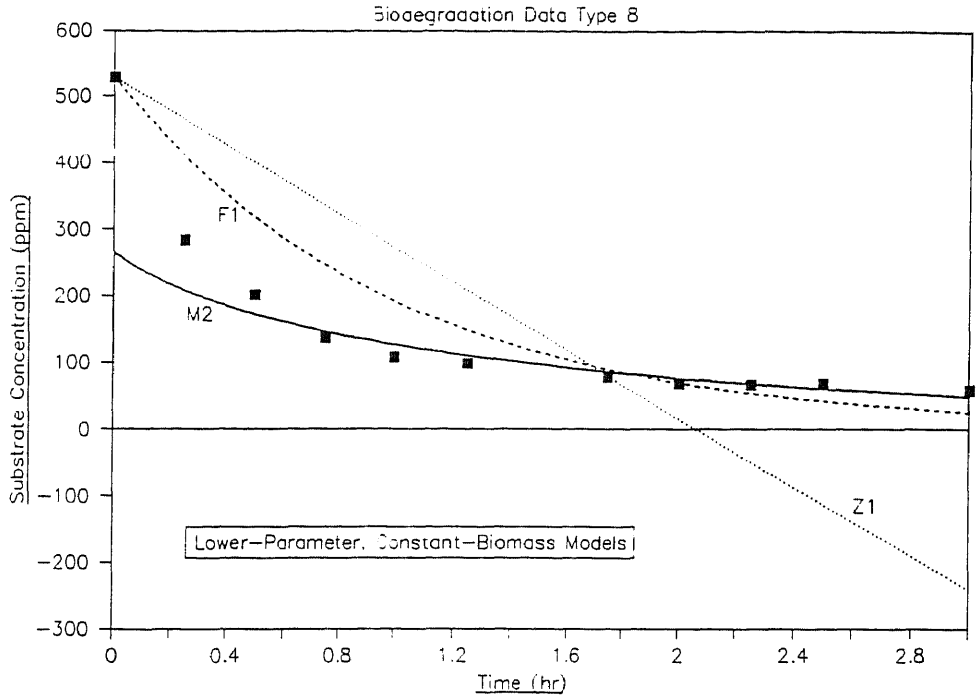
differences between the two sets of analyses: (1) the lag was included in the latter analysis accounting for the slightly lower value of μm, and (2) the authors did not report the value of Yc, requiring an estimated value (based on comparable substrate Yc values reported by them) to be used.

6.1.8 Data Type 8 (Greater-Than-First-Order Drop)

This biodegradation data type refers to those data sets which exhibit a definitively greater-than-first-order drop. This may be due to the simultaneous action of multiple substrate-elimination mechanisms (e.g., abiotic mechanisms, such as adsorption, volatilization and chemical oxidation), and not just biodegradation. Biodegradation of nth-order kinetics greater than one is not common. Therefore, description of this type of data as a separate "biodegradation" type in the pure sense of the term may not be correct. However, it is grouped and discussed separately here because of its occurrence in the literature, and the need to address concerns with respect to the modelling and utilization of these data for design purposes.

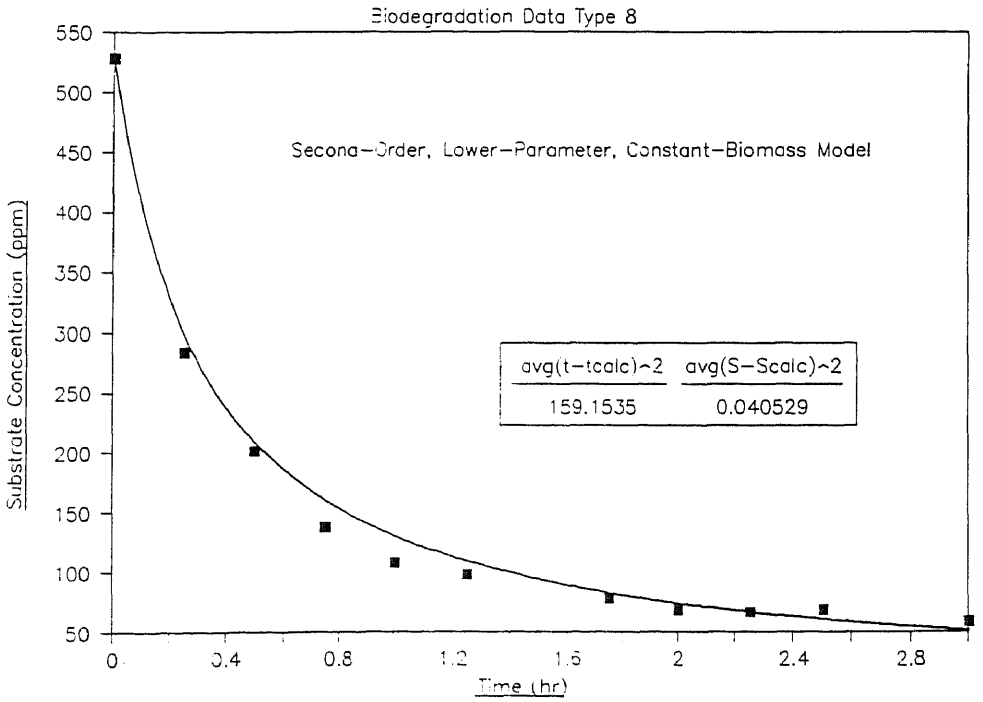
Figure 67 presents a data set measured by Chudoba, et al, which is of biodegradation data type 8. The constant-biomass models evaluated in this thesis on page D-24 are inappropriate for this specific case, as well as for this data type in general (refer to Figure 67 for a visual presentation of the Z1, F1 and M2 models). The Monod models are statistically best of those evaluated, but regress negative values of both

Figure 67



Source : Chudoba, J., Grau, P. & Ottova, V. (data set #1 shown on page D-24)

Figure 68



Source : Chudoba, J., Grau, P. & Ottova, V. (data set #1 shown on page D-24)

k and K for data of greater-than-first order (as mentioned previously in Section 6.1.2). Even with the negative rate constants, however, the Monod models are incapable of fitting data much greater in order than first. While the zero- and first-order models always regress positive rate constants, they are both worse in terms of fit than the Monod with the zero-order being incapable of modelling any curvature and the first-order underestimating the rate of drop.

Chudoba, et al, used a second-order model (as shown in Figure 68) to fit the data set shown in Figure 67. This data set is different from all the others evaluated in this thesis in that it is for more than one substrate (i.e., peptone and starch) with S being quantitated in terms of COD. Grau and Dohanyos[6], on the basis of numerous experiments and thorough theoretical analysis, proposed the following differential equation for multicomponent substrate-removal kinetics:

$$-dS/dt = k_n Bo(S/So)^n \quad ; (3)$$

where,

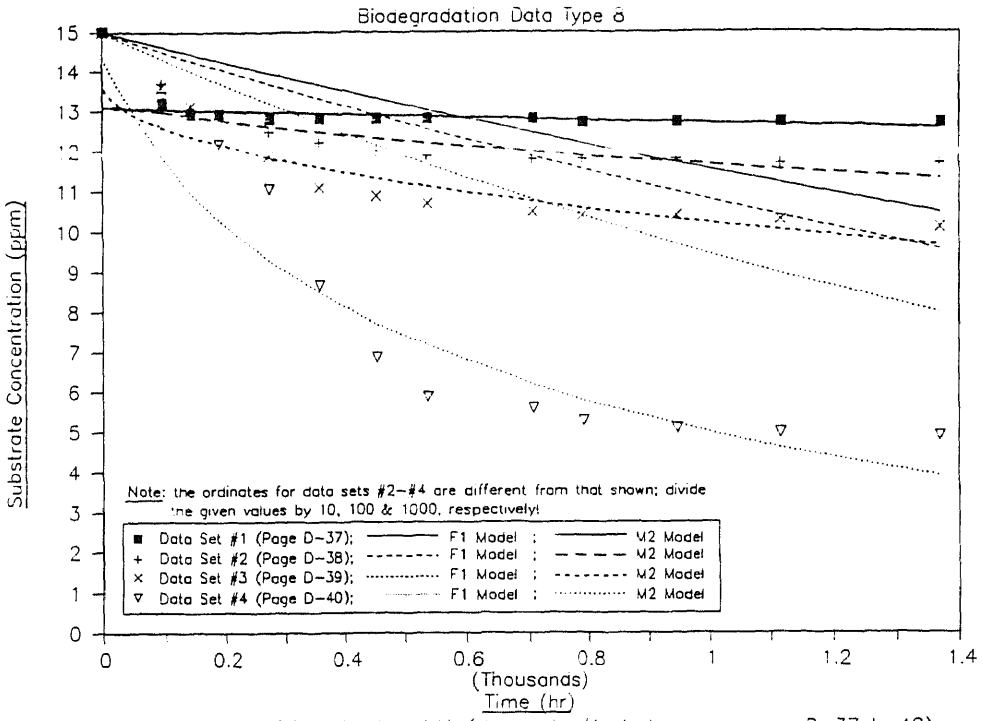
k_n = specific substrate-removal rate constant of the nth order.

n = formal order of the reaction.

Equation (3) applies when the microorganisms do not compete for the same substrate. It is uncertain as to whether the previous assumption is correct for this data set or whether other, unaccounted-for, abiotic removal mechanisms are responsible for the greater-than-first-order drop observed in the data since no mention was made by the authors as to the magnitude of the abiotic effects.

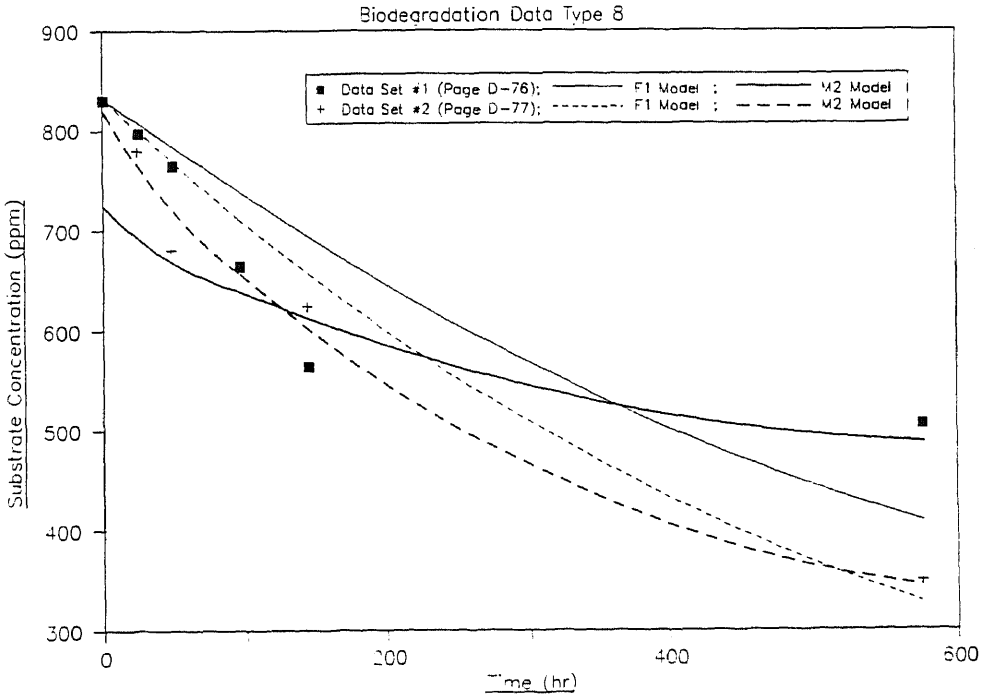
In addition to the data set shown in Figures 67 and 68, 13 more of the 124 mixed-culture data sets evaluated in this thesis are categorized as data type 8. These sets are all presented graphically in Figures 69-74 along with the corresponding F1 and M2 curves. All of these sets have the common characteristic of regressing negative values of both k and K for the Monod models (i.e., M2 and M3). Unlike the previously discussed data set, these sets are for single-substrate systems where the nth-order model presented as Equation (3) is not applicable. No generally-accepted kinetic theory is currently available to support the observed cases of nth-order biodegradation of greater-than-first order. The observed greater-than-first-order kinetics are regarded as artifacts of the data which may be attributed to any, or all of the following: (1) inaccurate measurements, (2) unaccounted-for, abiotic, substrate-removal mechanisms, (3) product inhibition resulting in a dramatic decrease in substrate-utilization rate which, in turn, results in the data set being interpreted as type 8, and (4) some other essential nutrient becomes limiting instead of the substrate which would have a similar effect to that of product inhibition.

Figure 69



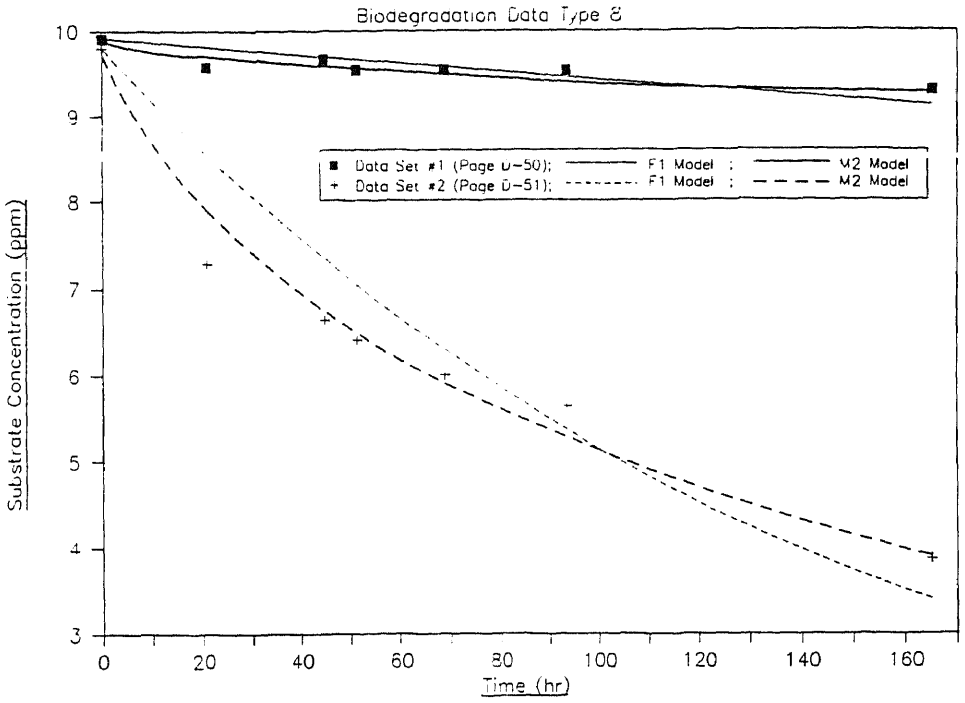
Source : Kaplan, D.L. & Kaplan, A.M. (data sets #1–4 shown on pages D-37 to 40)

Figure 70



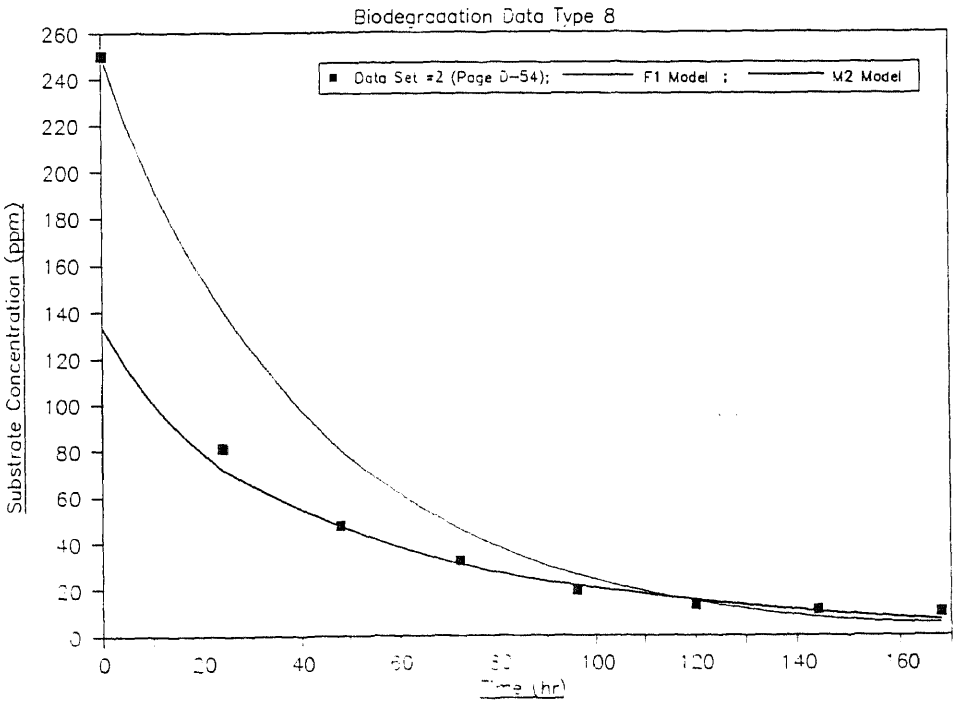
Source : Taylor, B.F. & Ribbons, D.W. (data sets #1 & #2 shown on pages D-76/7)

Figure 71



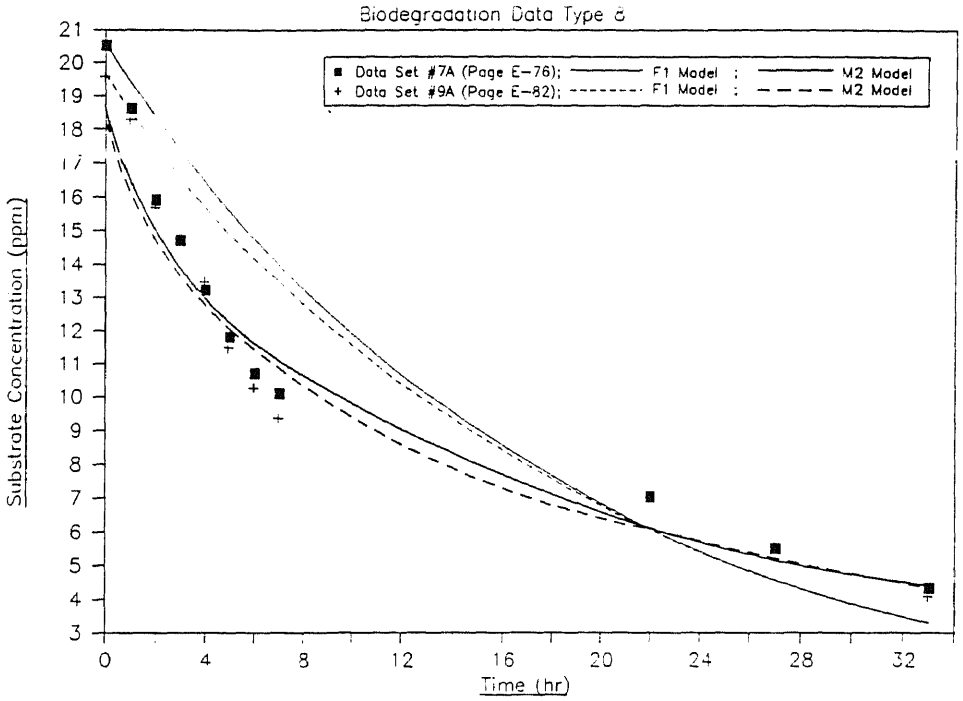
Source : Liu,D., et al (data sets #1 & #2 shown on pages D-50 & D-51)

Figure 72



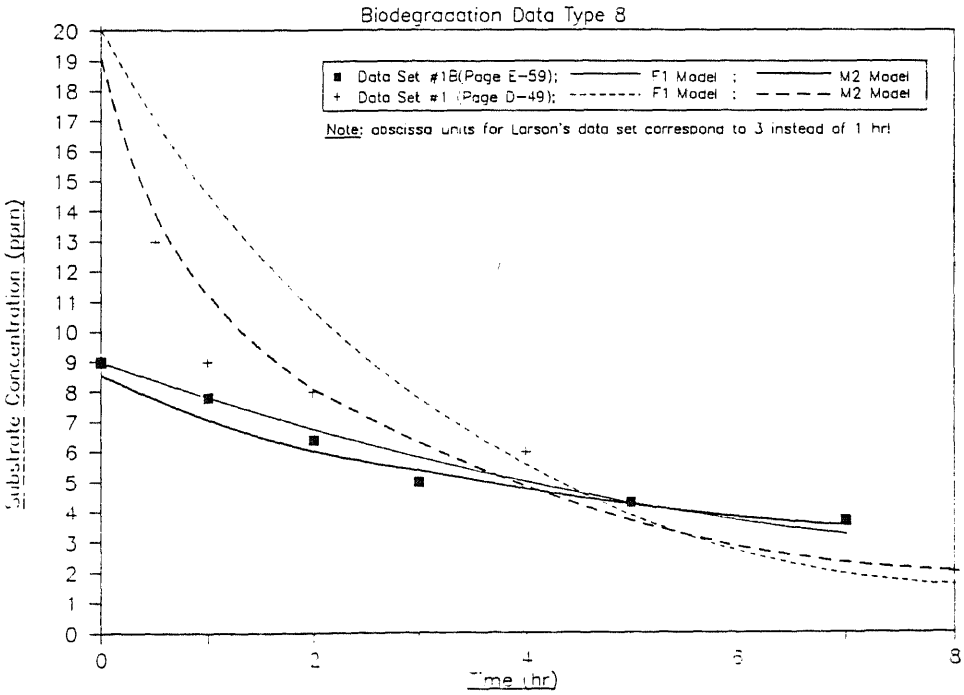
Source : Lyons, C.D., Katz, S. & Bartha, R.

Figure 73



Source : Naik Thesis (data sets #7A & #9A shown on pages E-76 & E-82)

Figure 74



■ Source : Naik Thesis (data set #1B on page E-59)
+ Source : Larson, R.J., Games, L.M. & King, J.E. (data set #1 on page D-49)

Figure 69 presents four data sets from Kaplan and Kaplan which are of type 8 primarily because of inaccuracies in the method which the authors used to determine S. Instead of measuring S directly, they radioactively labelled the substrate and quantitated the rate of biodegradation by detecting ^{14}C in traps as a function of time. Their questionable assumptions of biodegradation leading to complete mineralization (i.e., without any assimilation), and of the traps being 100% efficient, were not validated. The errors caused by these inaccurate assumptions in the back-calculated S vs t data likely account for the observed S levelling off at values higher than actual. Furthermore, the authors did not assess whether abiotic effects or product inhibition were contributing factors. It should be noted that the authors did evaluate Michaelis-Menten kinetics following manipulation of these data sets. They estimated the instantaneous reaction rate for each set and then regressed the obtained values vs. So for each set. They found the data to be first order with K>>S. Whereas the authors reduced the errors in their kinetic analysis via the data manipulation, the validity of the results obtained are no less questionable as abiotic effects were not addressed.

Figure 70 presents the data sets from Taylor and Ribbons. Both are interpreted as type 8 largely because of the last point in each being high. The missing points in the intermediate region of each set along with apparent data inaccuracy make these sets of no practical value from a kinetic analysis perspective.

Figure 71 presents two data sets from Liu, et al, for which the authors subtracted contributions due to abiotic effects based on control runs. While significant data scatter is present in both sets, it is apparent that S drops at a greater-than-first-order rate. The authors, however, erroneously regressed these data to first-order models (as they also did for a set shown in Figure 65 and discussed in Section 6.1.7 on page 106). They regressed first-order rate constants of 0.0004/hr and 0.0053/hr for data sets #1 and #2, respectively. Based on a comparison with the corresponding regression results shown on pages D-50 and D-51, it appears that the authors used the F2 version of the first-order model for their analyses.

The data set shown in Figure 72 from Lyons, et al, is not corrected for the effect of abiotic mechanisms although the authors did attempt to assess the relative contributions of evaporation, auto-oxidation and adsorption. Even after correcting the data for the above-mentioned abiotic effects, however, the set is still clearly greater than first order. The authors' techniques for quantification of abiotic effects were not validated, and it is possible that the adsorption effect, as a result, was underestimated. The other data set from this literature source was categorized as type 2 (refer to Figure 21 in Section 6.1.2). The system used for this data set had a much lower level of biomass (i.e., pond water vs sludge) which would account for the contribution of the adsorption effect being significantly reduced in its case.

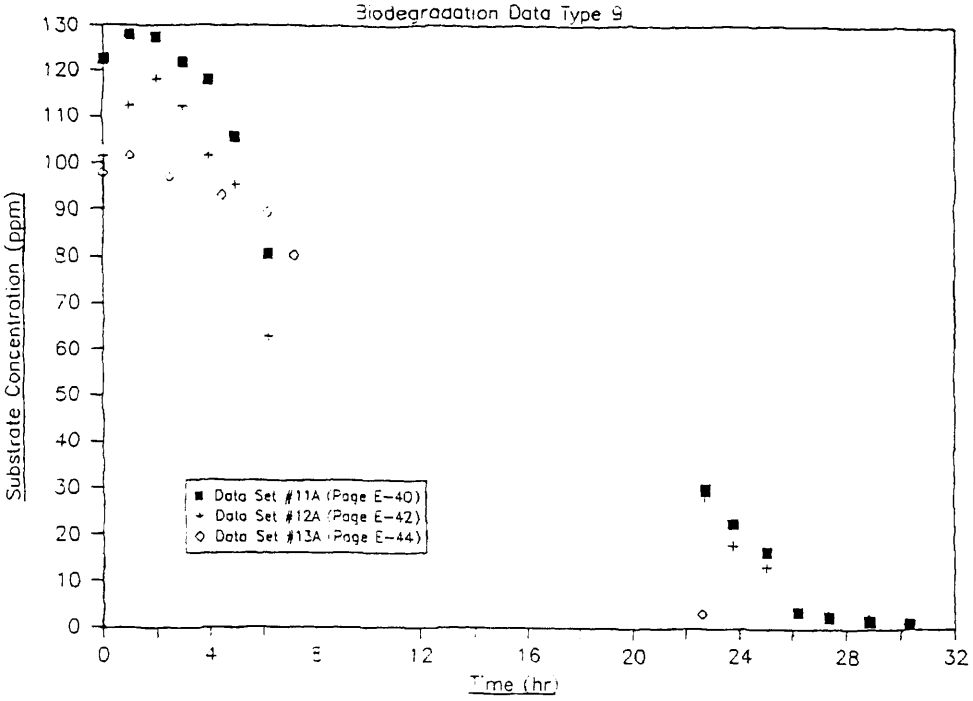
It should be noted here that the variable-biomass models are capable of fitting greater-than-first-order kinetics with positive rate constants when negative yield constants are used. This was briefly discussed in Section 6.1.4 (refer to Figures 40, 42 and 44). Negative values of Yc, however, while potentially possible (i.e., during periods of net cell death), are not the norm.

6.1.9 Data Type 9 (Miscellaneous)

The remaining 12 data sets for batch-reactor, mixed-culture systems (not previously discussed in Sections 6.1.1 through 6.1.8) are covered in this section under the broad category of miscellaneous. These sets are classified as type 9 for the most part because of their poor quality data (e.g., high scatter, missing points and/or apparently erroneous measurements). As a result, the data sets are either different from types 1-8, or intermediate between two or more types, with selection of the correct one not being able to be made conclusively.

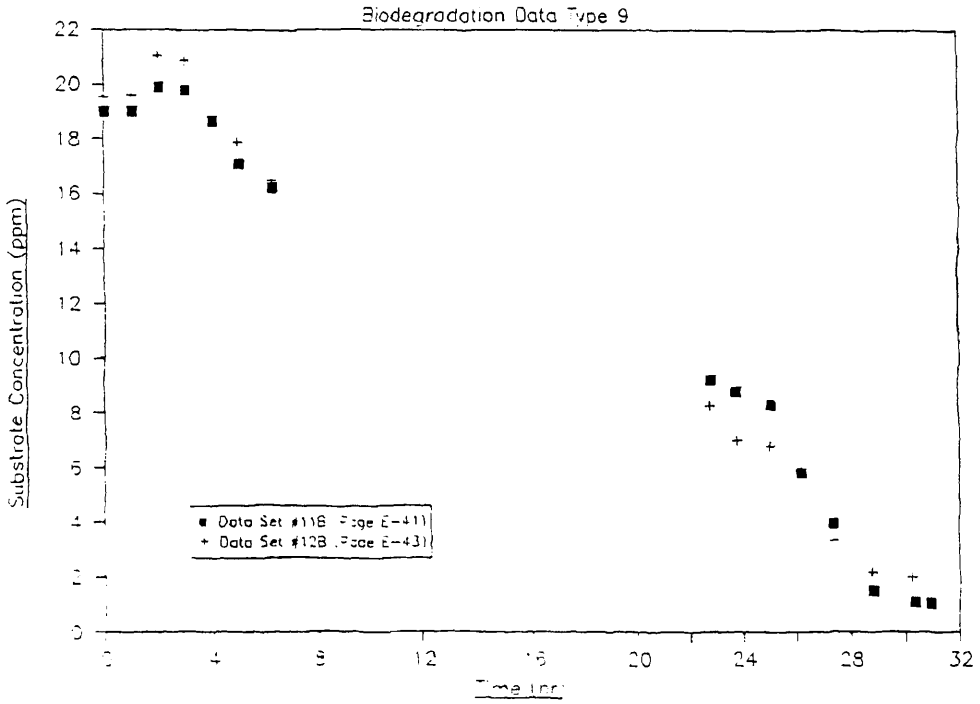
Figures 75 and 76 present 5 data sets from the Gonnabathula thesis which are of type 9 because of the very poor quality of the data. The combination of high data scatter and omission of data points in the central (i.e., overnight) time period makes selection of the specific data type impossible. Kinetic analysis of these sets yields little of practical value. The only

Figure 75



Source : Gonnabathula Thesis (phenol as substrate in mlss)

Figure 76



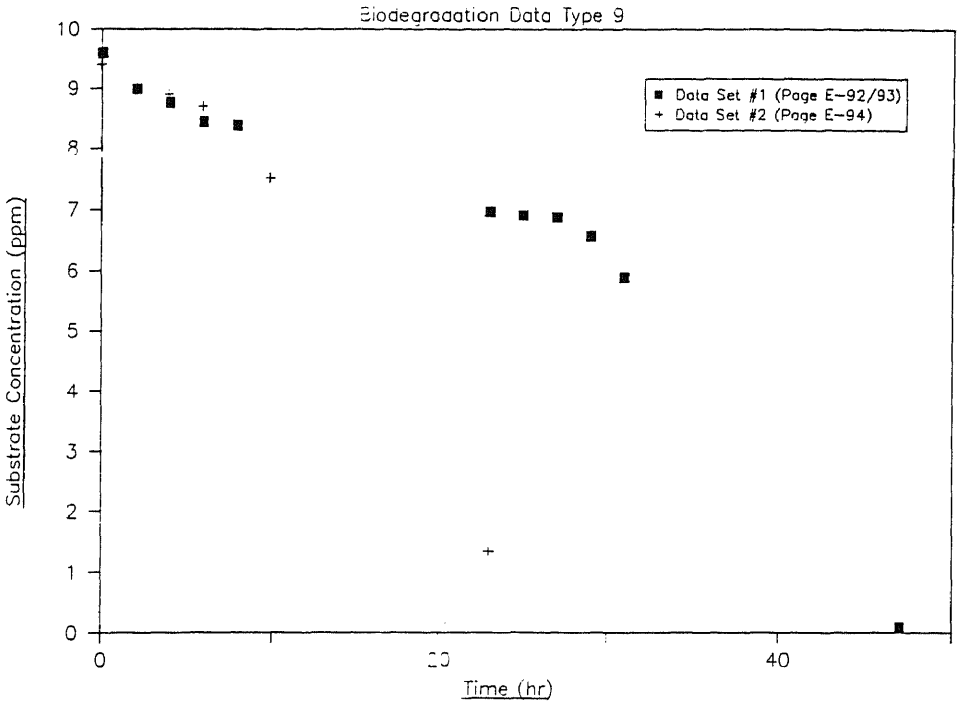
Source : Gonnabathula Thesis (nitrobenzene as substrate in mlss)

information of value to be deduced from these sets is that: (1) lags are present, and (2) biodegradation down to certain levels takes place within given time periods. Knowledge of the S vs t profiles, however, cannot with any reliability be predicted from these data.

Figure 77 graphically presents 2 data sets from Pak's thesis which show slow but steady degradation prior to the last point of each set. The last point of each set is much lower than expected which may be due to either some unexplained change in the culture which results in a dramatic increase in its activity or it may just be an artifact of the analytical method. Without data from the intermediate, overnight periods, however, the true nature of these sets cannot be determined.

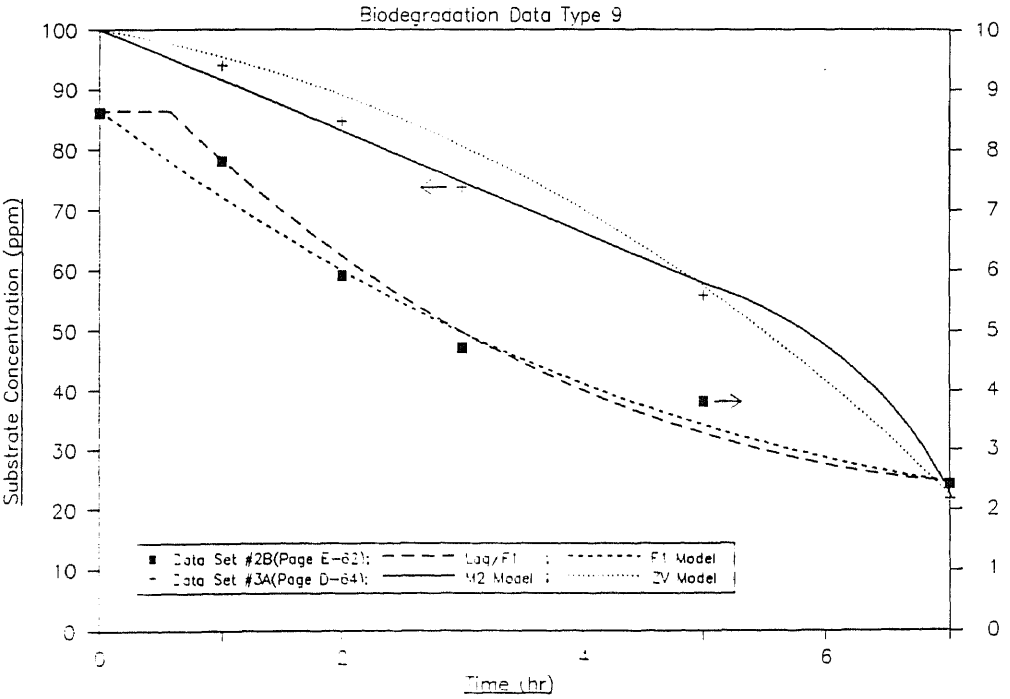
Figure 78 shows 2 data sets from the Naik thesis which are of better quality than the preceding sets in this section. Data set #2B exhibits sufficient scatter, however, to make conclusive interpretation of its specific data type difficult (e.g., it can be any of types 2,3,4,5,7 or 8). Figure 78 shows the F1 model with and without lag for comparison purposes. Data set #3A is shown to be very well represented by the M2 model with a negative value of K (because of the apparent downward bend in the data). Whereas the ZV model can fit a downward bend with a positive rate constant, it is incapable of fitting a shape like this, with a linear drop followed by a sudden

Figure 77



Source : Pak Thesis (2,6-dichlorophenol in activated sludge)

Figure 78



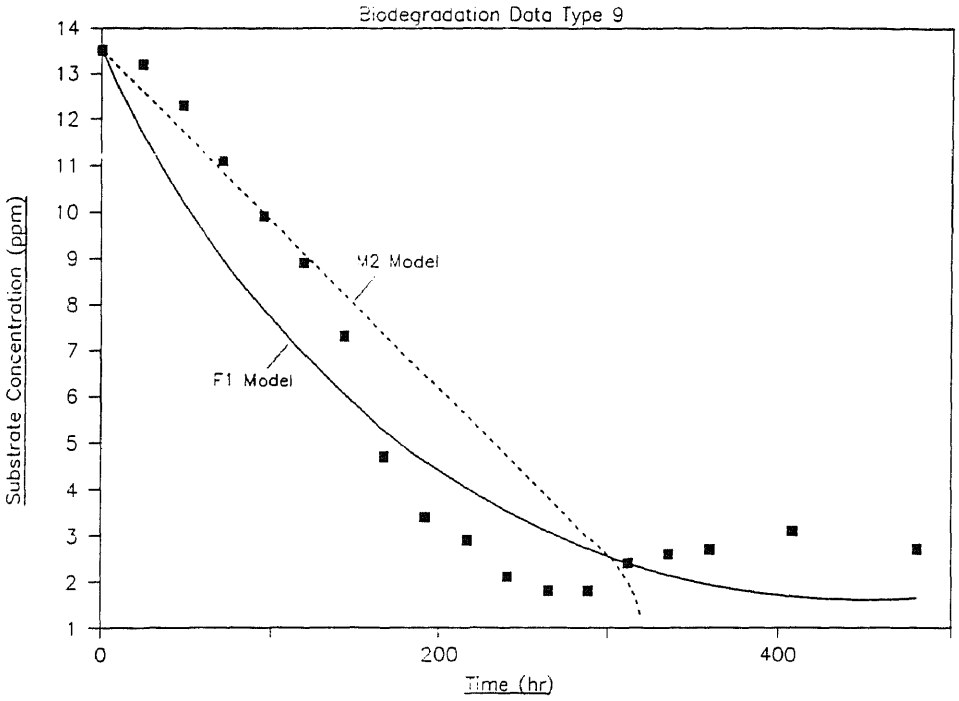
Source : Naik Thesis (substrates : unacclimated sludge)

increase in the biodegradation rate. A hypothetical ZV model is provided in Figure 78 for comparison purposes (Bo was selected for an assumed Yc of 0.5 so as to minimize $\Sigma(t\text{-}tcalc)^2$). Additional data points in the latter region of this set would have provided more information with which to better interpret its kinetics. As presented, however, the integrity of the last data point is questioned.

Figure 79 presents a data set from Blanchard, et al, which appears to demonstrate MV kinetics in the initial half of the set. The second half of the set exhibits the anomalous effect of S increasing with t, which is likely an artifact of the authors' analytical procedure. The authors radioactively labelled the methylcellulose substrate, then measured the radioactivity in the supernatant as a function of time, and related the detected ^{14}C-concentration to S. The observed apparent increase in S may have been the result of the release of ^{14}C into the supernatant as part of soluble by-products of endogenous respiration. Blanchard, et al, summarized the results of their experiment with a zero-order rate constant to represent the rate of substrate utilization. Representation of the data as zero-order is a poor approximation, but the apparent inaccuracy of the data negates the practical utility of an accurate kinetic analysis.

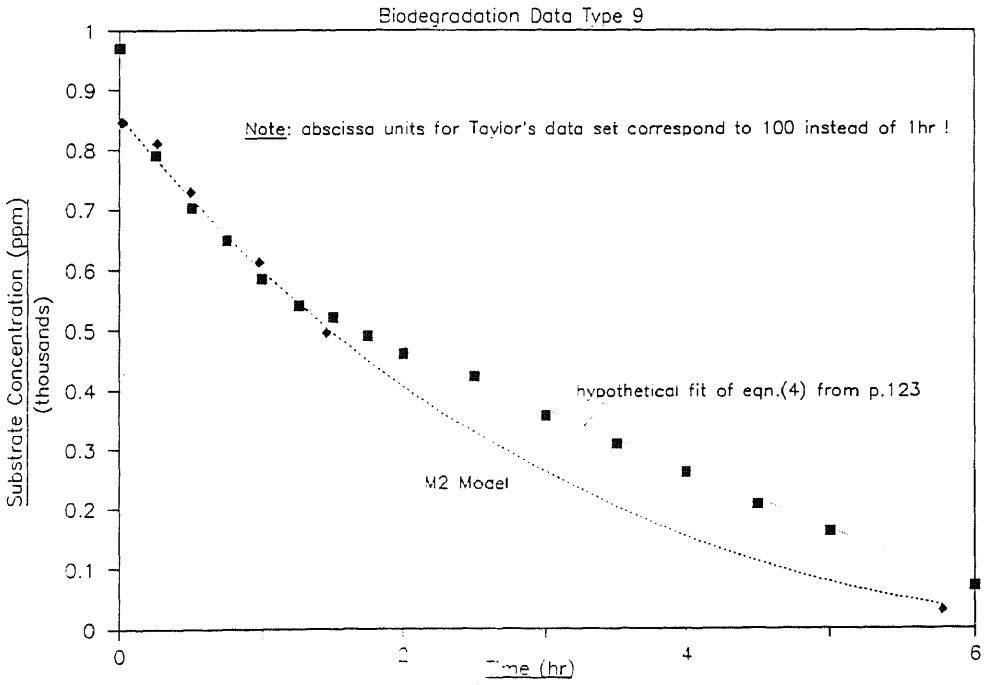
The remaining 2 data sets categorized under type 9 are presented in Figure 80. The set from Cech, et al, is unusual in that the initial drop is rapid and of first-order nature before transition to a slower, zero-order drop. The authors attributed the

Figure 79



Source : Blanchard, et al (refer to data set #1 on pages D-20/21)

Figure 80



■ Source : Zech, et al (data set #1 on pages D-22/23)
◆ Source : Taylor, B.F. & Ribbons, D.W. (data set #3 on page D-78)

initial rapid drop to the accumulation capacity of the involved microorganisms for the substrate. They used the following model based on storage and accumulation processes to represent the data:

$$-dS/dt = Ko + K_1 Sra * \exp(-K_1 t); \quad (4)$$

where,

Ko = zero-order rate constant due to storing processes

K_1 = first-order rate constant due to accumulation processes

Sra = apparent volumetric accumulation capacity

Equation (4) may be a suitable approach for modelling the combined effects of biodegradation and adsorption simultaneously. The models on pages D-22 and D-23 show MV to yield negative values of k and K while M2 and M3 yield positive rate constants. The MV model would have yielded positive rate constants if a negative value of Yc were used.

The data set in Figure 80 from Taylor and Ribbons is well represented by the Monod model (i.e., type 3) but appears to exhibit a possible lag based on the second data point being higher than predicted, which would result in this set being classified as type 7. Lack of data in the initial portion of this set makes conclusive categorization difficult. Based on the relatively small magnitude of the alleged lag relative to the overall biodegradation

time frame, however, it has little practical impact on the fitting of the data unless interest lies specifically with the initial portion of the data set. It should be noted that the two other data sets from Taylor and Ribbons were categorized as type 8 (refer to Figure 70). The lack of data points in the region preceding the last point of each set places too much reliance from the kinetic analysis perspective on the integrity of the last point of each set. Whereas data sets #1 and #2 were interpreted as greater-than-first order and data set #3 as less-than-first order, the interpretation by the models is determined by the accuracy of the last point of each set and may just be the result of experimental error and not necessarily reality.

6.2 Batch Reactor Data--Single Culture Systems

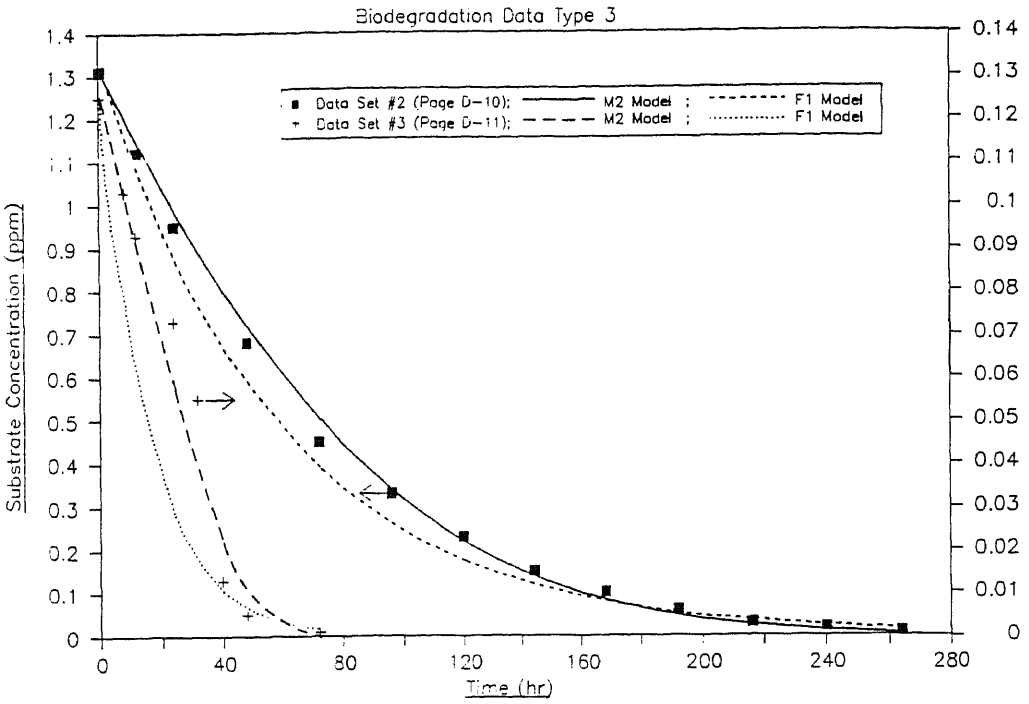
Whereas the bulk of the batch reactor data sets evaluated in this thesis are for mixed-culture systems, a significant proportion of those extracted from the literature (i.e., 16 of 54) involved single-culture systems. While single-culture systems are not common in industrial wastewater treatment operations, nor in natural environments, certain species may dominate the response of a heterogeneous population (e.g., activated sludge) to a give substrate. Study of single-culture systems usually results in more reliable kinetic data than mixed-culture systems (providing abiotic substrate-removal mechanisms are accounted for) because: (1) the active biomass concentration can be more readily determined; and (2) there is no shift in population during the course of an experimental run. A higher proportion of the bacteria are active

in substrate-specific, single-culture systems than in mixed-culture systems. Measurement of kinetic data, however, should be performed at relatively high food-to-microorganism ratios (i.e., S/B) to avoid conditions of endogenous respiration where the percentage of active biomass is noted to decrease substantially.

The discussion of all of the data sets for single-culture systems will be conducted within this section as the total number is tractable and the characteristics of each individual data type (specifically with respect to modelling by the constant- and variable-biomass versions of the zero-order, first-order and Monod kinetic models) were alrady covered in detail in Sections 6.1.1 through 6.1.9.

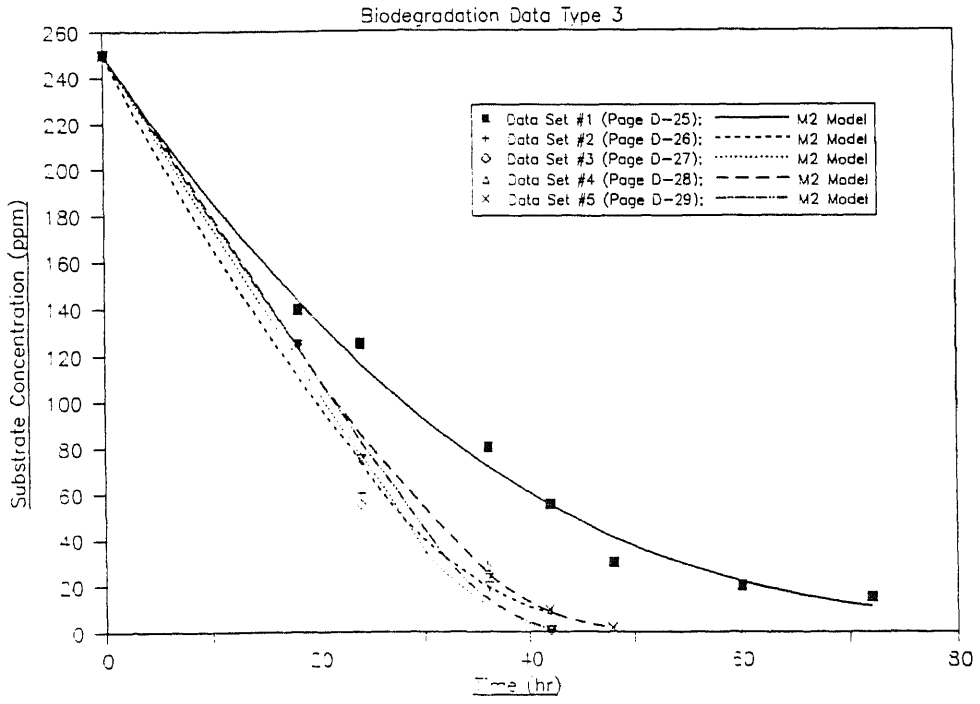
The bulk of the single-culture systems investigated in this thesis (i.e., 9 of 16) are categorized as biodegradation data type 3. Figure 81 presents 2 of these data sets which were extracted from an article by Allard, et al. The M2 models are shown to well represent both cases; the corresponding F1 models are presented for comparison purposes and clearly show the reaction order in each case to be less than one. The increased scatter in data set #3 vs #2 is the result of decreased analytical accuracy at lower S values. The objective of the study by Allard, et al, was to assess the impact of discharges of chloroguaiacols into the environment. Even though the authors noted the data sets to be concentration dependent, they estimated pseudo-zero order rate constants from linear portions of the curves and converted

Figure 81



Source : Allard, A.S., et al (3,4,5-trichloroguaiacol in strain 1395)

Figure 82



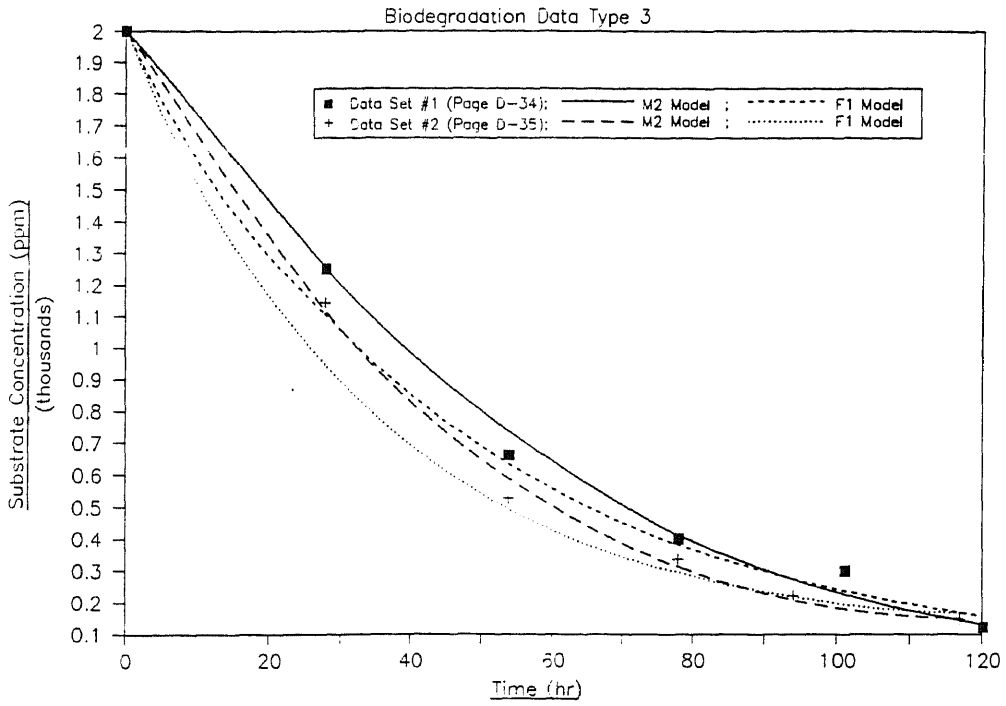
Source : Garbara, S.V. & Rotmistrov, M.N. (HMDA in B.subtilis)

them into specific rates by dividing by the cell density. The variable-biomass models were not evaluated in Appendix D for these 2 sets for the following reasons: (1) adequate biomass data were not presented by the authors, (2) no variable-biomass effect was evident in the data sets, and (3) the authors classified the biomass as non-proliferating and stated that B was virtually constant throughout both experiments. The authors also noted difficulty in obtaining accurate biomass measurements due to problems with plating the dense cultures which were used.

Figure 82 presents 5 data sets of type 3 from Garbara and Rotmistrov which are well represented by the M2 models. The article's primary purpose was to study the oxidative and degradative activity of B.subtilis, which utilizes hexamethylenediamine (HMDA) as the sole nitrogen and carbon source, and the effect of clay minerals on these processes. Biomass measurements were not presented by the authors nor were kinetic analyses performed.

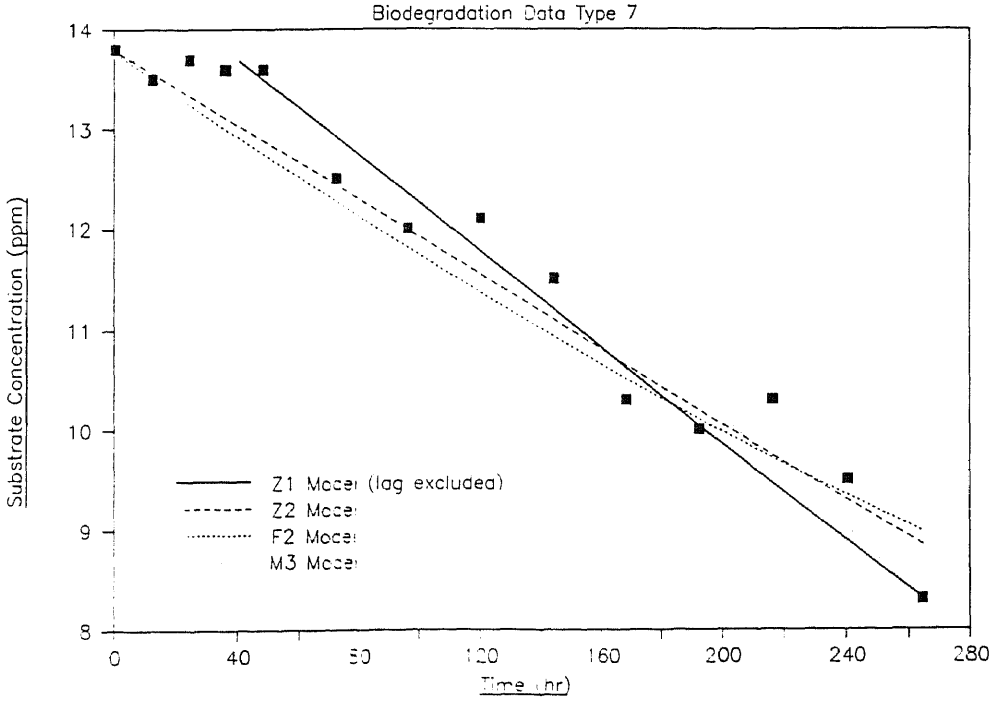
The remaining 2 single-culture data sets of type 3 were extracted from Ilyalendinov, et al, and are presented in Figure 83. Both sets are slightly less than first order and are shown to be well represented by the M2 models. Whereas variable-biomass data were provided by the authors for both cases, Yc was far from constant indicating that the assumption of exponential growth throughout the S range covered was not valid; the variable-biomass models were, therefore, not valid and, hence, not evaluated. Data set #3 from

Figure 83



Source : Ilyalendinov, et al (alpha-methylstyrene as substrate)

Figure 84



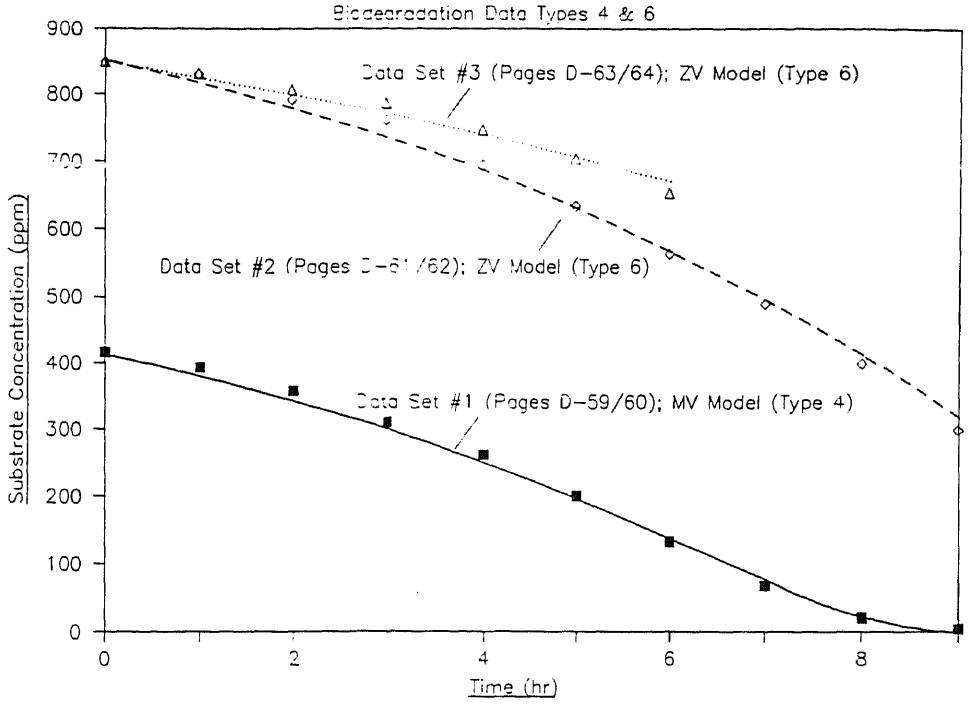
Source : Allard, A.S., et al (refer to data set #1 on page D-9)

Ilyalendinov, et al, was classified as type 4 (refer to the figures on page 65); data sets #1 and #2 may also possibly be of type 4, but the lack of information available on the data sets (i.e., lack of points in the initial region, no report of analytical accuracy, and lack of reliable variable-biomass data) does not substantiate such a conclusion.

The other 7 of 16 single-culture data sets studied in this thesis are of types 4, 6 and 7. Figure 84 shows data set #1 from Allard, et al, to be of type 7. Because of the relatively high data scatter and the small S range covered (and because the lag is short relative to the overall biodegradation time), none of the models shown on page D-9 result in bad fits. While the Monod models are the best of those shown on page D-9, they both result in negative values of K due to the apparent downward bend in the S vs t data. Figure 84 visually shows the constant-biomass, zero-order model (with the lag excluded) to be the best for this data set.

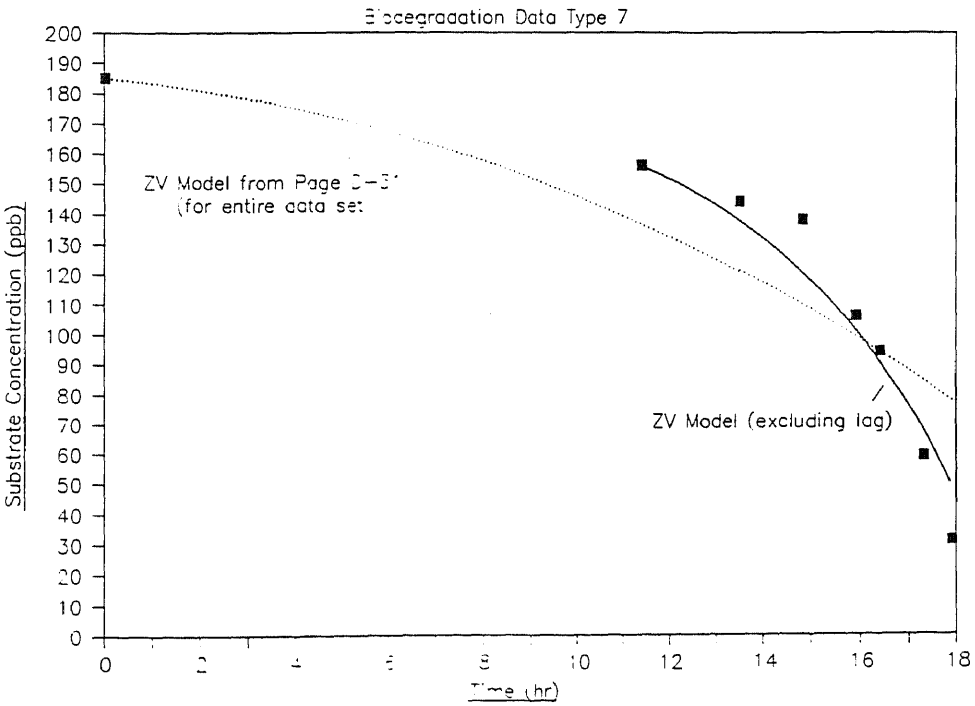
Figure 85 shows 3 data sets from Radhakrishnan and Sinha Ray (for phenol in B.cereus) to be well-represented by the variable-biomass models utilizing the biomass data measured by the authors using a Klett-Summerson photoelectric colorimeter. Data set #1 is of type 4 and is shown to be very well-represented by the MV model from page D-60; the measured values of Bo and Yc result in a near optimum fit for the MV

Figure 85



Source : Radhakrisnnan, [illegible] & Sinha Ray, A.K. (phenol in B.cereus)

Figure 86



Source : Hill, G.A. & Robinson, C.W. (refer to data set #1 on pages D-30 & 31)

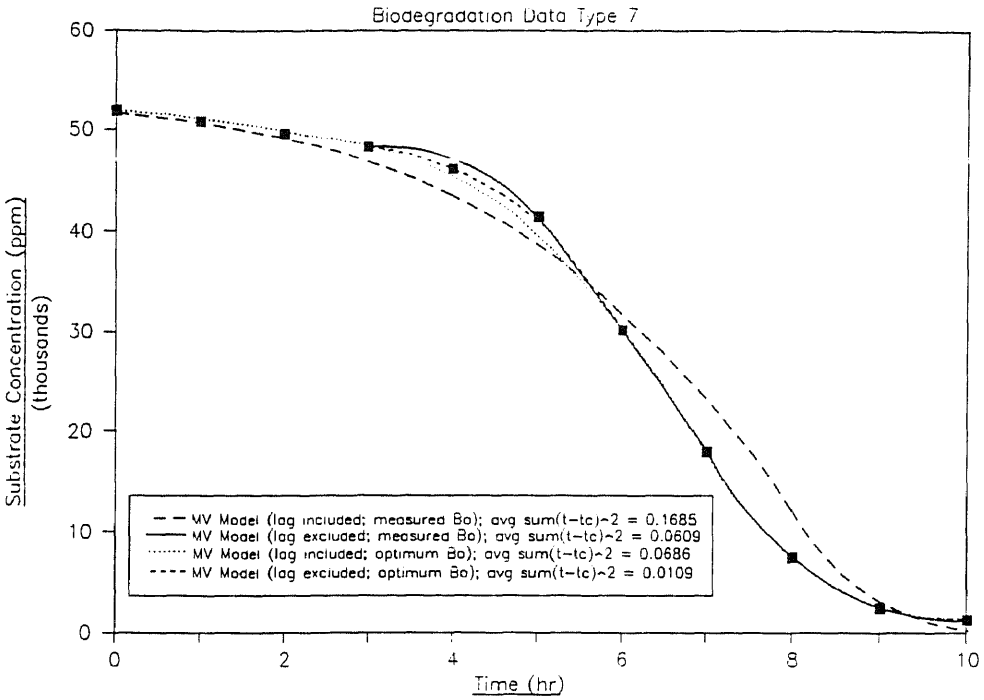
model. The predicted curve has a slightly smaller variable-biomass effect than actually observed which may be due to the measured Bo being slightly higher than the actual viable biomass concentration; this is likely since the photoelectric colorimeter measures the total (not active) biomass concentration. Data sets #2 and #3 are both of type 6 and are shown to be fairly well represented by the ZV models from pages D-62 and D-64, respectively. In each case, however, the measured value of Bo is higher than the actual active biomass concentration resulting in the variable-biomass models underpredicting the variable-biomass effects observed. The higher-than-actual Bo (active biomass concentration) values account for the MV models on pages D-62 and D-64 regressing negative values of K in order to best fit the data sets. For the values of Yc used in data sets #2 and #3, the values of Bo would have to be less than 95 ppm and 40 ppm (instead of the measured values of 143 ppm and 155 ppm), respectively, for the MV models to regress positive values of K.

The remaining 3 single-culture data sets exhibit lags and are classified under the category of biodegradation data type 7. Figure 86 presents the first of the 3 which was extracted from an article by Hill and Robinson. Figure 86 shows the ZV model from page D-31 (which includes the lag portion in the regression analysis) and the corresponding ZV model for which the lag portion was excluded from the regression analysis. While better performance is apparent in the latter

case, both models underpredict the observed variable-biomass effect because of an overprediction of Bo, which is the result of the biomass measurement technique used (i.e., optical density) being a measure of the total, and not active, biomass concentration. It should be noted that the variable-biomass models are not theoretically valid for the data set shown on page D-31 since they assume that the biomass is in the exponential growth phase over the entire range considered, which is apparently not the case here (i.e., the lag is present). The authors excluded the lag from their kinetic analysis in which they studied the more complex substrate-inhibition models (e.g., Haldane, Andrews and Aiba-Edwards equations).

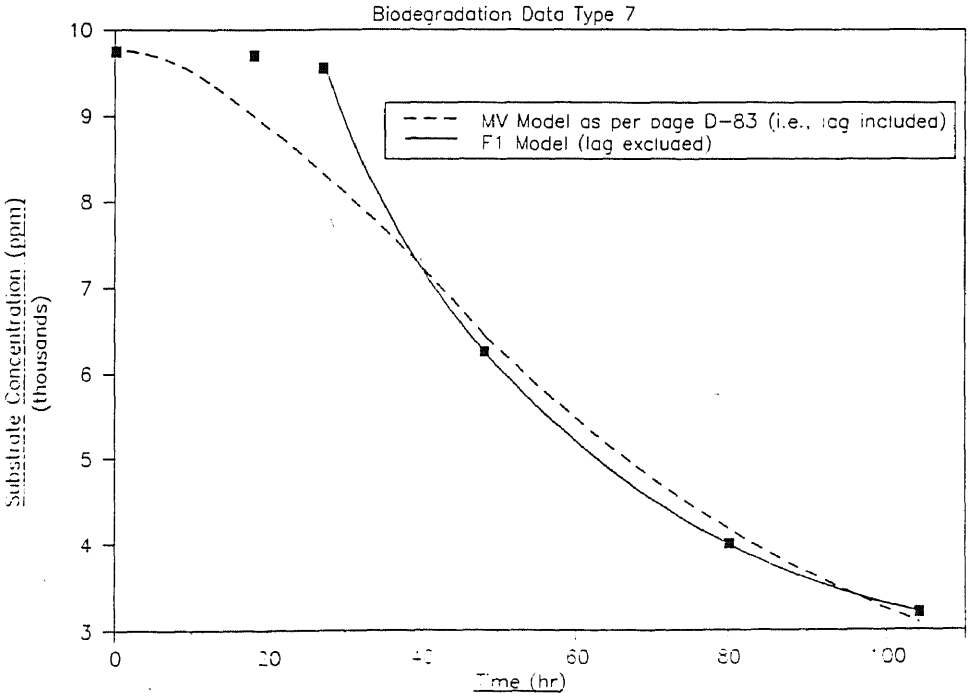
The second single-culture data set of type 7 was extracted from Tanner and is shown in Figure 87 along with the following 4 different MV curves: (1) same as shown on page D-75 (using entire set and measured value of Bo), (2) same as 1 except that the lag (i.e., initial 3 data points) was excluded from the regression analysis, (3) same as 1 except that the optimum value of Bo was used (i.e., Bo was selected so as to minimize $\Sigma(t\text{-}tcalc)^2$), and (4) same as 2 except that the optimum value of Bo was used. Examination of these 4 curves yields the following conclusions: (1) even though the lag is slight with a gradual transition into the exponential growth phase, allowing reasonable representation of the entire data set by the MV model, markedly better results are obtained when excluding the lag portion from the regression

Figure 87



Source : Tanner, R.D. (data set #1) ; refer to pages D-74 & D-75

Figure 88



Source : Wong, P.T., Lu, D. & Dutka, B.J. (refer to data set #1 on p.D-82/83)

analysis, and (2) while biomass determination via optical density measurements yields reasonable results in this case, the variable-biomass effect is again underpredicted as a result of the method measuring total (instead of active) biomass concentration. Tanner presented this data set as preliminary support for a proposed, mechanistically-more-complex model.

The last batch reactor data set to be discussed for single-culture systems is from Wong, Liu and Dutka (refer to Figure 88). The transition from lag to biodegradation is too sharp to be well represented by the MV model shown on page D-88. Best results are obtained by neglecting the lag during the kinetic analysis. The first-order model, for example, is shown to well fit the remaining points. No kinetic analysis was performed by the authors of this data set.

6.3 Continuous Stirred-Tank Reactor Data

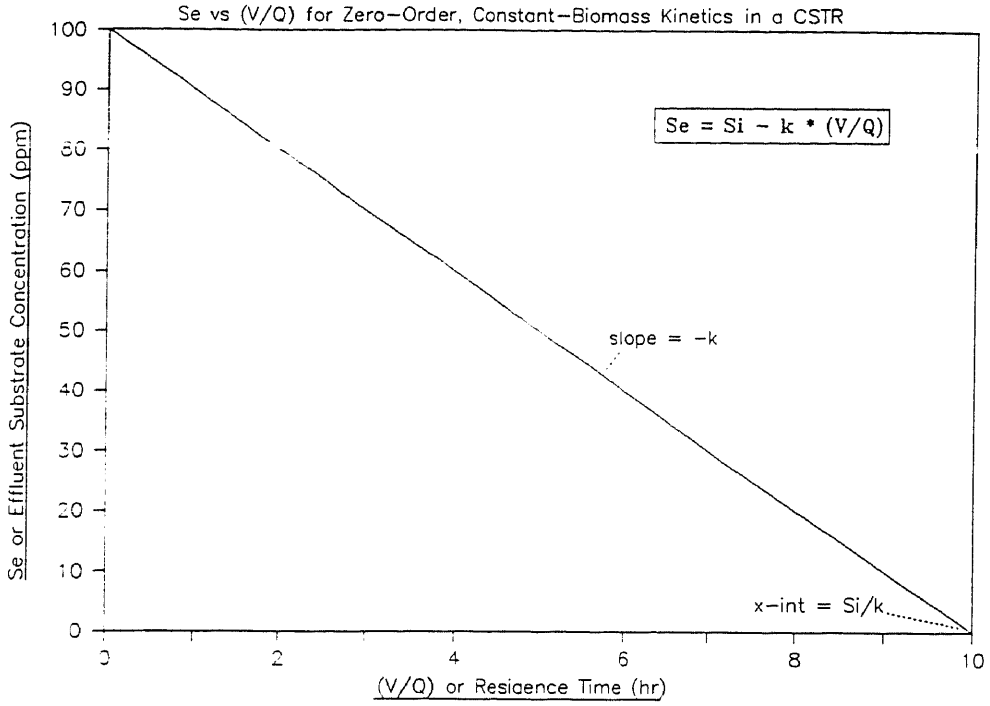
Only 8 of the 148 biodegradation data sets studied in this thesis were obtained using continuous stirred-tank reactors (i.e., CSTRs). This is attributed to the fact that CSTRs are more difficult to set up, run and obtain reliable measurements. The use of CSTRs for the study of biodegradation poses certain advantages, however, over batch reactors: (1) the kinetic analysis is simpler involving only algebraic manipulations (vs. calculus for batch reactor data analysis), and more importantly (2) almost all industrial and municipal wastewater treatment facilities operate in the continuous mode (as opposed to batch). Laboratory studies in CSTRs, therefore, provide a better manner with which to measure and predict the biodegradation reactor's performance on large scale.

The kinetic expressions derived in Appendix B are for ideal CSTR behavior and require that the following assumptions be met by laboratory-scale units in order for the equations to be theoretically valid: (1) substrate concentration, Se, vs. residence time, (V/Q), measurements are made under steady-state conditions, (2) constant reactor volume is maintained, and (3) the composition of substrate and biomass is uniform throughout the reactor. The first and second assumptions can generally be met. However, even with effective mixing and aeration, wall growth can nullify the third assumption, unless the reactor walls are periodically scrubbed down. For biodegradation kinetics which are typically of fractional order, the assumption of perfect (micro) mixing for design purposes will result in the prediction of higher substrate converions than that of the segregated-flow (macromixing) approach.[7] This, in turn, can result in the undersizing of a plant-scale, wastewater-treatment reactor. The segregated flow approach, however, is experimentally and analytically more difficult and the resulting improvement in results may, in many cases, only be marginal.

The characteristic S vs t curves shown in Figure 1 on page 20 for batch-reactor data sets are not applicable to CSTRs. The corresponding characteristic effluent substrate concentration, Se, vs residence time, (V/Q), curves for CSTRs are shown in Figures 89-94 for the zero-order, first-order and Monod expressions presented in Table 2 on page 15. The variable-biomass versions shown in Figures 90, 92 and 94 assume Be to equal (Bi + Yc(Si-Se)), which for sterile feeds (i.e., Bi = 0) reduces to (Yc(Si-Se)). These relationships do not apply when either wall growth occurs or sludge is recycled (i.e., they are valid only for a chemostat). It should be noted that both the constant- and variable-biomass, lower-parameter models allow regression to include data points in which Si is varied in addition to (V/Q). The Se vs (V/Q) curves, however, can only be graphically presented for the case in which Si is held constant.

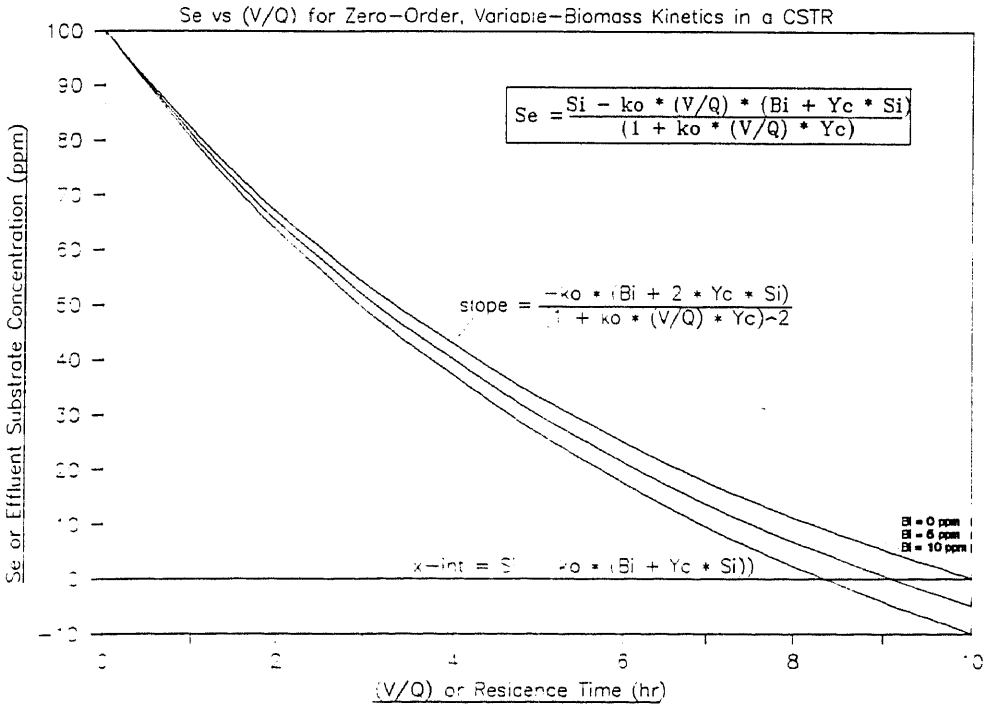
Figure 89 shows the zero-order, constant-biomass relationship for a CSTR to be analogous to that for a batch reactor. The model in both cases predicts substrate concentration (Se or S) to drop linearly with time (i.e., residence time for a CSTR), and for conversion to be complete after a fixed time period (i.e., Si/K or So/K). The Se vs (V/Q) curve for zero-order. variable-biomass kinetics in a CSTR, however, is different from that for the batch reactor (e.g., compare Figure 90 with Figure 39). Figure 90 shows the rate of conversion to decrease with residence time before ultimately becoming complete at a time equal to Si/(ko(Bi+YcSi)).

Figure 89



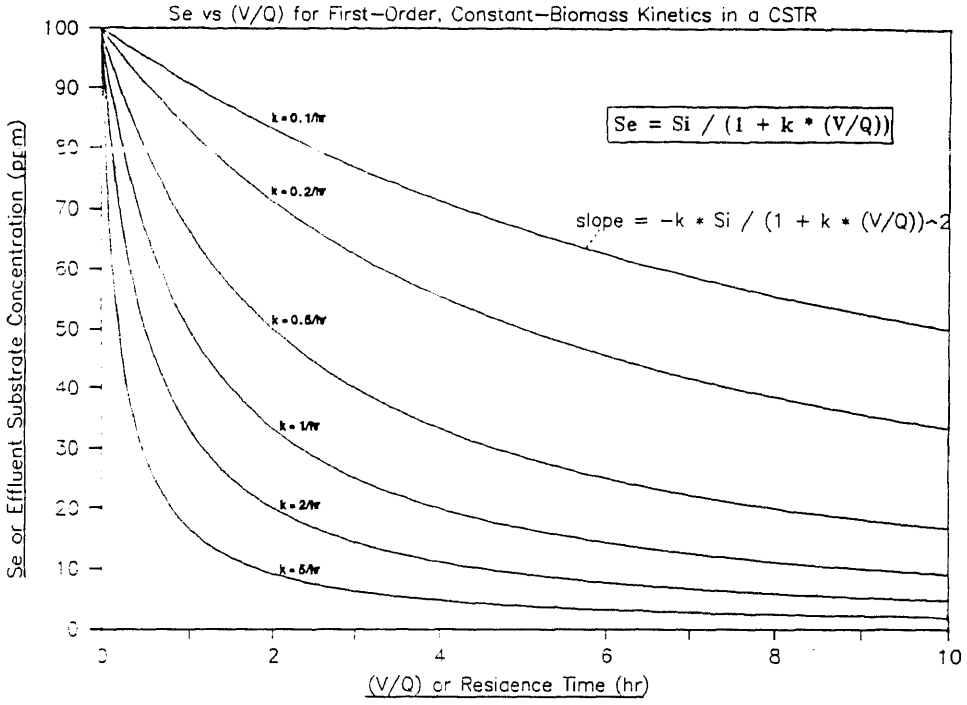
Assumptions: Si=100 ppm & k=10 ppm/hr

Figure 90



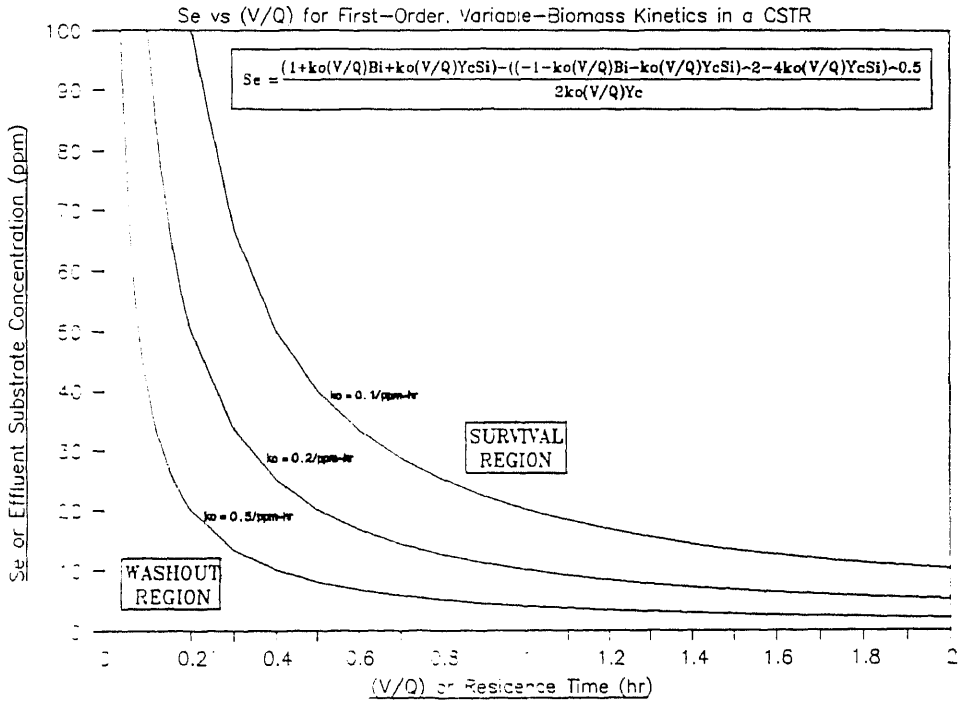
Assumptions: Si=100 ppm, ko=0.2 ppm/ppm-hr & Yc=0.5

Figure 9.1



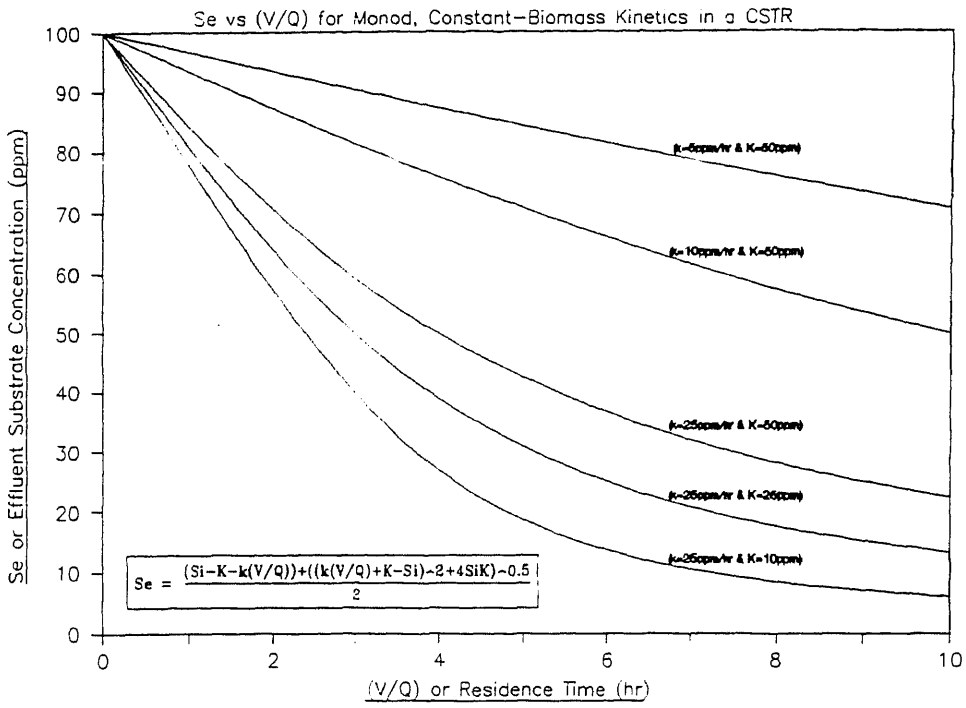
Assumptions: Si=100 ppm & k varies as shown

Figure 9.2



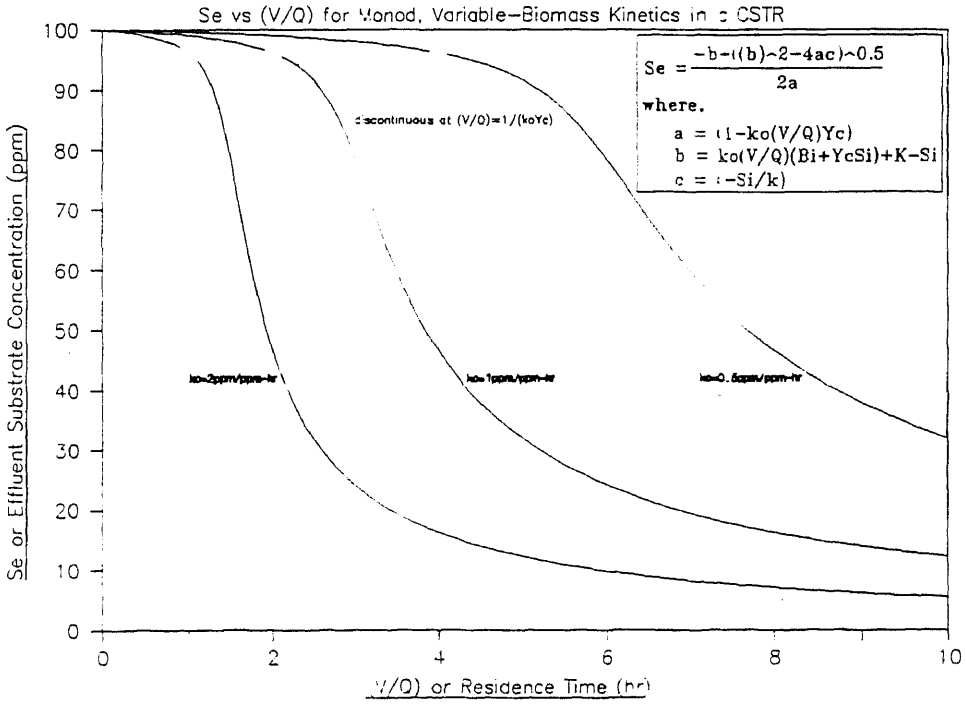
Assumptions: Si=100 ppm, Bi=0(sterile feed), Yc=0.5 & ko varies as shown

Figure 93



Assumptions: Si=100 ppm while k & K vary as shown

Figure 94



Assumptions: Si=100 ppm, Bi=1 ppm, Yc=0.5, K=50 ppm & ko varies as shown

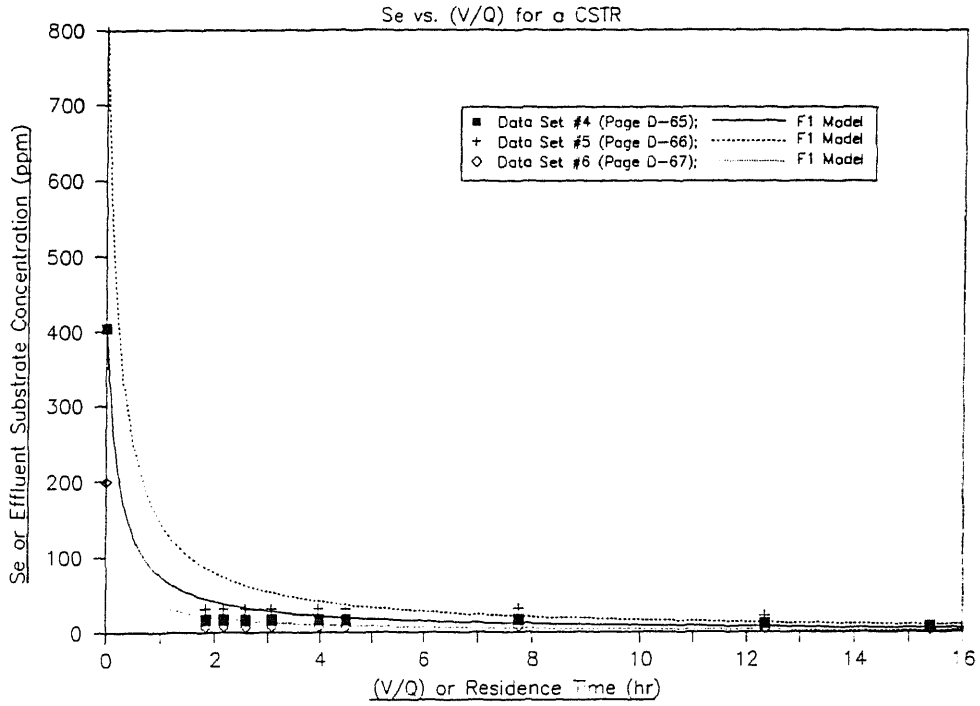
Figures 91 and 92 graphically present the characteristic Se vs (V/Q) curves for the case of first-order kinetics in a CSTR. Of particular interest in Figure 92 is that (for the kinetic parameters arbitrarily selected) no conversion of substrate is obtained below certain residence times when operating under steady-state conditions. This is due to the physical phenomenon known as washout and occurs when the rate of loss of biomass in the effluent exceeds its generation rate. Figure 92 shows that washout occurs at progressively lower residence times as the rate of substrate utilization increases.

The characteristic Se vs (V/Q) curves for Monod kinetics in CSTRs are graphically shown in Figures 93 and 94. The curves are visually analogous to those for ideal batch reactors. It should be noted that the MV curves in Figure 94, however, are discontinuous for a CSTR at values of (V/Q) equal to 1/(koYc). This is not an actual physical phenomenon but rather a mathematical artifact of the quadratic equation used.

The 8 CSTR data sets studied in this thesis were extracted from 4 different articles. The discussion of the results from each article is handled separately within this section because of inherent differences in CSTR operation by the different authors.

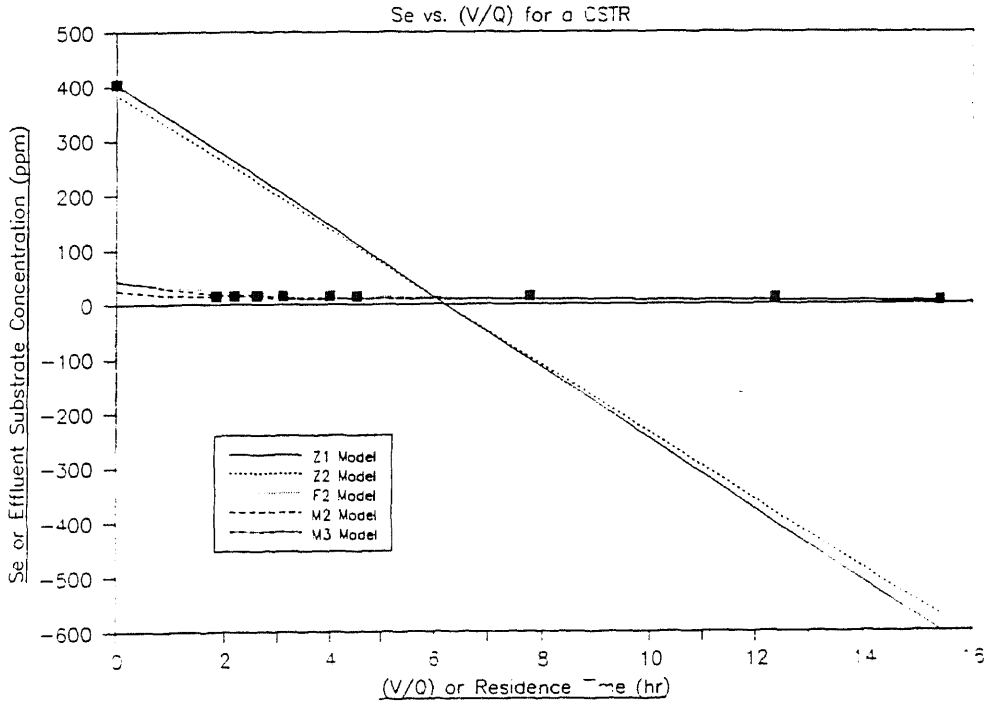
Figure 95 presents 3 CSTR data sets which were extracted from Radhakrishnan and Sinha Ray. Whereas the authors presented biomass concentration data for these sets, the variable-biomass models were not

Figure 95



Source : Radhakrishnan, I. & Sinha Ray, A.K. (phenol substrate in B.cereus)

Figure 96

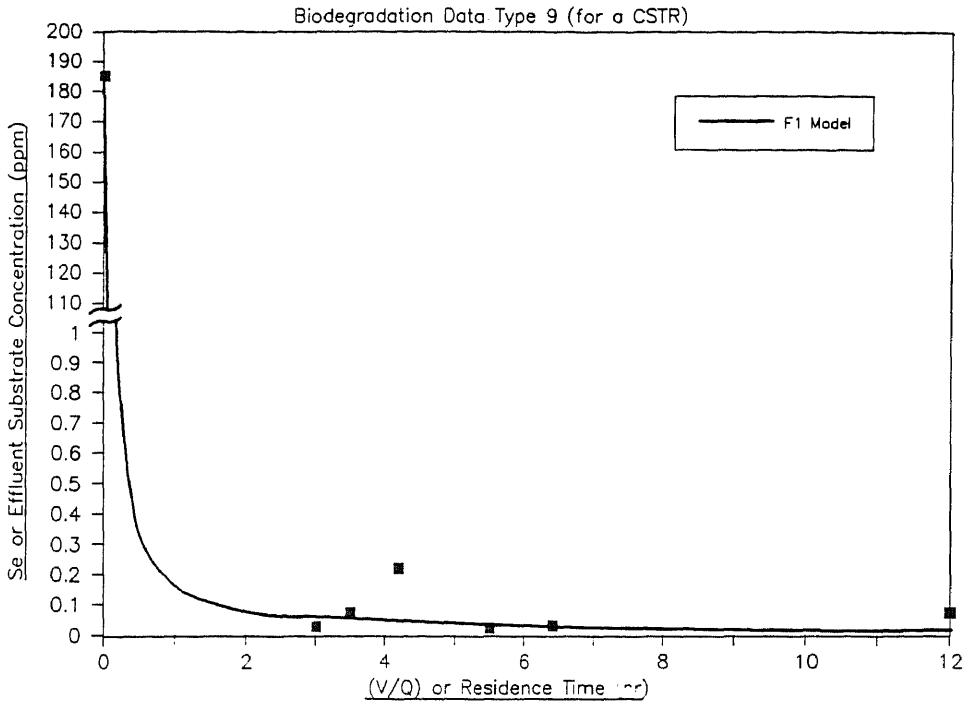


Source : Radhakrishnan, I. & Sinha Ray, A.K. (data set #4 from page D-65)

evaluated in Appendix D because the measured biomass concentration was constant for each set over the range of residence times covered. The F1 curves are visually the best of the models evaluated and are shown for each of the 3 sets in Figure 95. For comparison sake, Figure 96 shows the other 5 regressed curves for only one of the 3 sets since the general performance characteristics for all 3 are comparable. The M2 and M3 models regress negative values of both k and K in each case because of the data apparently dropping at greater-than-first-order rate (i.e., biodegradation data type 8), which is analogous to batch reactor behavior. None of the models evaluated in this thesis are capable of adequately representing these sets. The authors noted that Se and Be remained constant over the residence times covered possibly because of sensitivity limitations on the analytical methods. They also noted that neither the Michaelis-Menten relation nor the Tissier equation (i.e., $\mu = \mu m(1-\exp(\text{constant}*Se))$) hold for the measured data. Measurements for lower residence times would have provided greater insight into the kinetic behavior of these data systems. It should be noted that the authors made no mention as to the validation of the perfect mixing assumption of their CSTR via residence time distribution studies and, as such, the validity of the data for kinetic analysis purposes must be questioned.

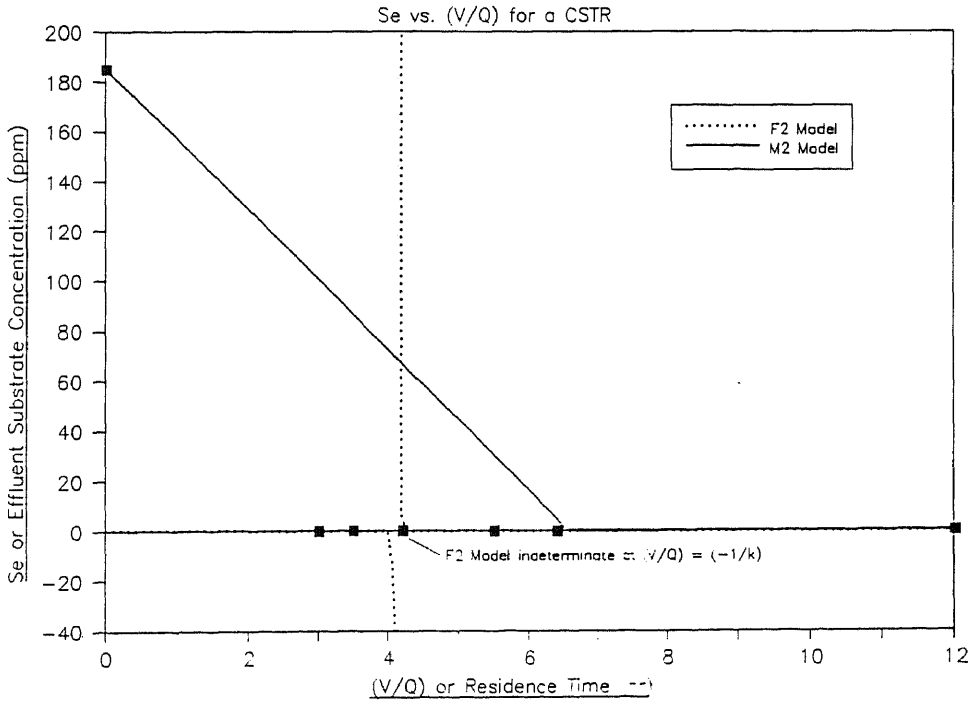
Figure 97 presents a data set from Hill and Robinson which is analogous to those in Figure 95 in that Se is very low and virtually constant (within the apparent accuracy of the analytical method) over the residence time tested. Again, F1 is the visually best model and is

Figure 97



Source : Hill, G.A. & Robinson, W.R. (data set #2 on pages D-32 & D-33)

Figure 98



Source : Hill, G.A. & Robinson, W.R. (data set #2 on pages D-32 & D-33)

presented in Figure 97. Unlike the data sets in Figure 95, however, this data set causes all of the Monod models to regress negative values of K only (i.e., k is positive in each case). This is attributed to the data point at a residence time of 4.2 hr which has a value of Se that is an order of magnitude higher than the others (refer to pages D-32 and D-33). Not only does this abnormally high value of Se cause the Monod models to regress negative values of K, but it also causes the F2 model to regress a negative value for k. Figure 98 graphically presents the M2 and F2 curves for this data set.

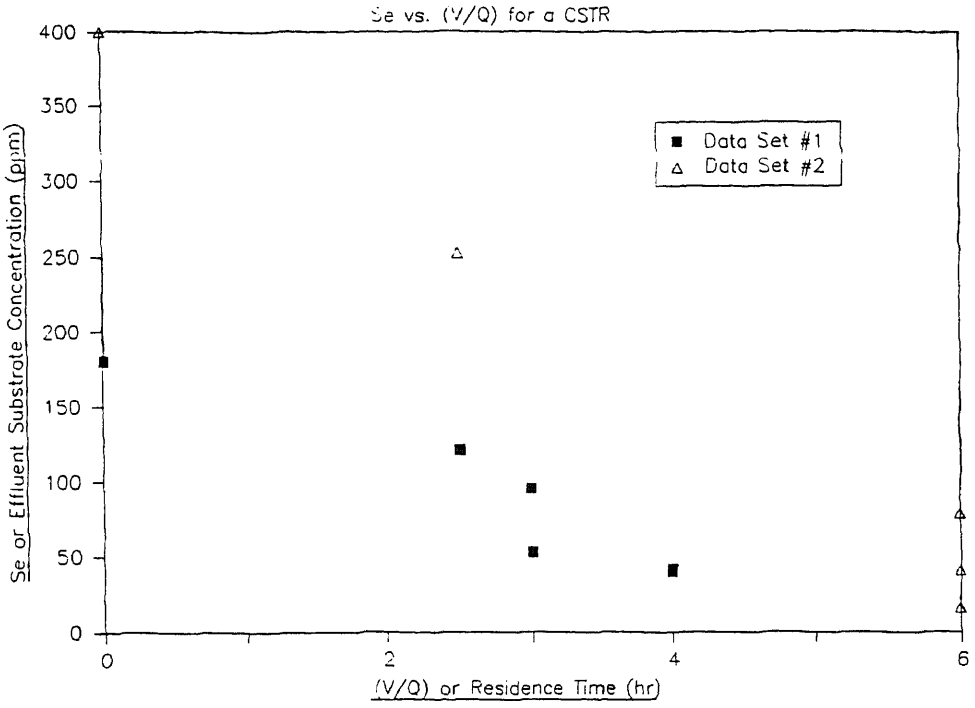
Hill and Robinson performed residence time distribution studies to confirm that their laboratory CSTR exhibited perfectly mixed behavior in the liquid phase over the range of feed and aeration rates used. The authors, however, did not confirm whether measurements were truly made under steady-state conditions. They stated that their measurements may only have been transient phenomena as their runs often had to be cut short because of observed wall growth. The lack of model-predicted response in Se by the authors (i.e., they evaluated substrate-inhibition models) was attributed by them to be due to either small variations in the feed rate or undetected, localized wall growth. Wall growth has long been known to affect measurement of kinetic parameters and process stability.

It should be noted that Hill and Robinson used sterile feed (i.e., Bi=0) and measured Be, which is theoretically equal to Yc(Si-Se), directly. The measured values of Be varied only slightly as the variable-biomass models closely approximated the lower-parameter, constant-biomass models. Because Be did, however, vary (even if only slightly) from data point to data point, and not exactly as per the relationship Yc(Si-Se), the Se vs (V/Q) plot does not result in smooth curves for the variable-biomass models with this data set (i.e., Se becomes a function of Be in addition to (V/Q)).

The remaining 4 CSTR data sets to be discussed are from 2 articles with the same principle author (i.e., Beltrame, P.). CSTR operation was reported to be the same in both cases. Sterile feed (i.e., Bi=0) was used along with sludge recycle such that the measured value of Be did not conform to the theoretical value of Yc(Si-Se). Whereas the assumption of steady-state behavior was confirmed by the authors through repeated measurements, no mention was made of their checking the validity of the assumption of perfect mixing in their laboratory set-up.

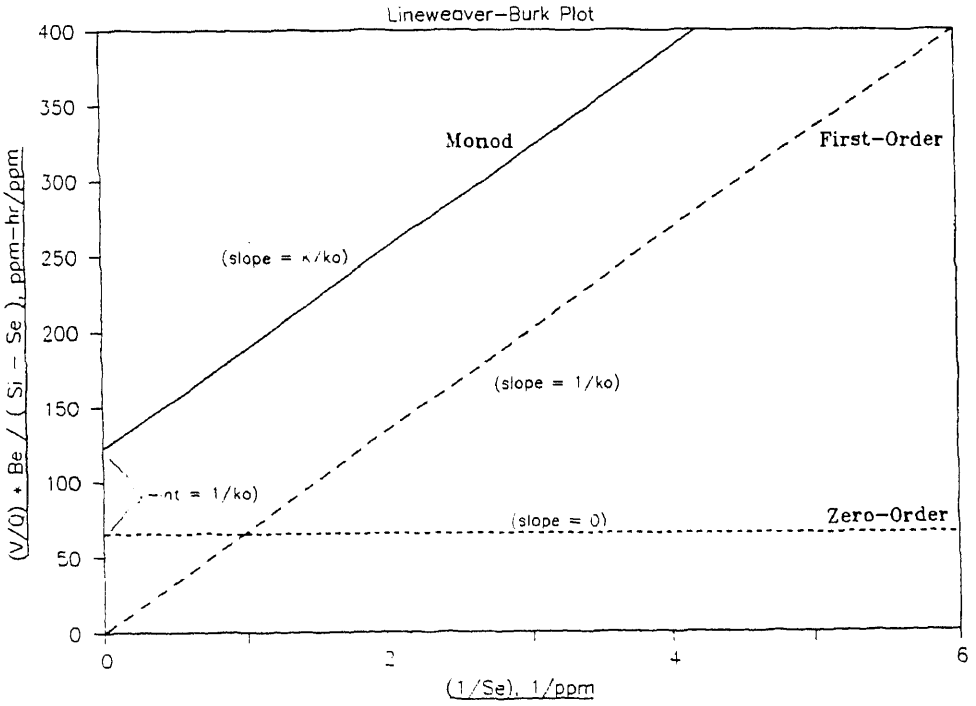
Figure 99 presents the Se vs (V/Q) plot for 2 CSTR data sets from Beltrame, P., et al (1984). The observed scatter in both data sets is due to significant variations in Be measurements throughout the runs (refer to pages D-13 and D-15). Because Be varies independently of Si and (V/Q) for these data sets due to the authors' use of sludge recycle, plots of Se vs (V/Q) are of no practical value here. For these cases, the Lineweaver-Burk plot (i.e., a plot of ((V/Q)Be)/(Si-Se) vs (1/Se))

Figure 99



Source : Beltrame, P., et al (1984); data sets #1 & #2 on pages D-12..D-15

Figure 100



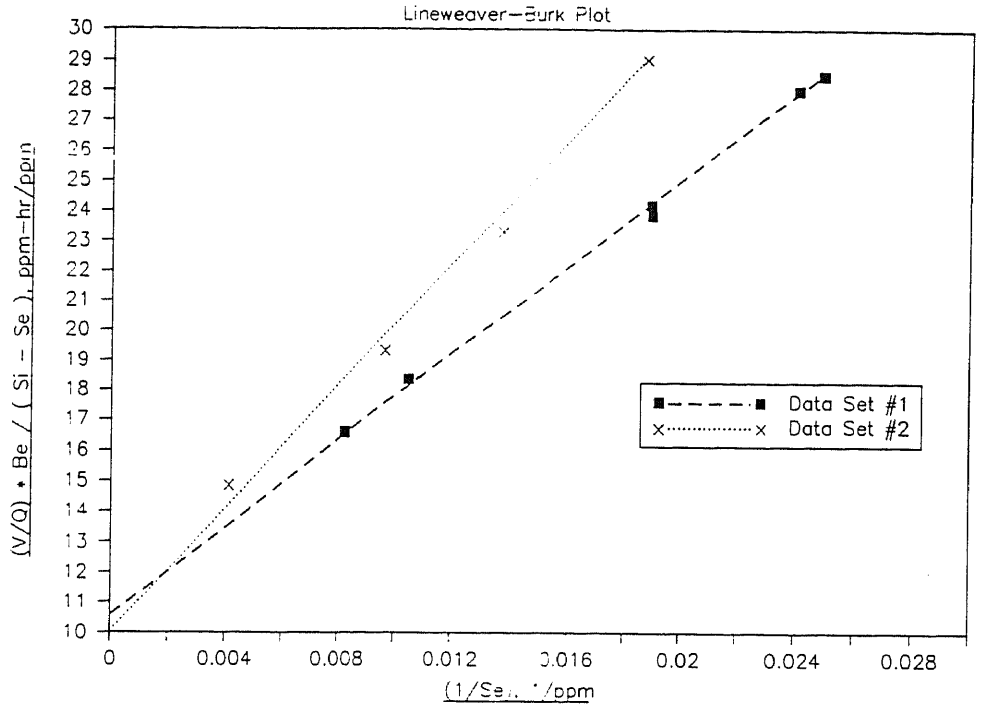
is preferred. Figure 100 shows the expected characteristic linear relationships of a Lineweaver-Burk plot for zero-order, first-order and Monod kinetics. Data sets #1 and #2 from Figure 99 are shown to be well represented by the Monod model on the Lineweaver-Burk plot in Figure 101. The regression results for these 2 data sets on pages D-12 through D-15 show the MV model to be best. M2 and M3 regresses negative values of both k and K while F2 regresses negative values of k for both data sets. Be is seen to vary too much from data point to data point (due to sludge recycle) for the data sets to be well-represented by the constant-biomass models.

The regressed results from pages D-13 and D-15 for the MV models are in good agreement with those performed by the authors. A comparison is provided below:

	Results from Appendix D		Results from Article	
	ko (hr^{-1})	K (ppm)	ko (hr^{-1})	K (ppm)
Data Set #1	0.0935	66.35	0.094±0.003	67±2
Data Set #2	0.0997	98.20	0.095±0.007	91±9

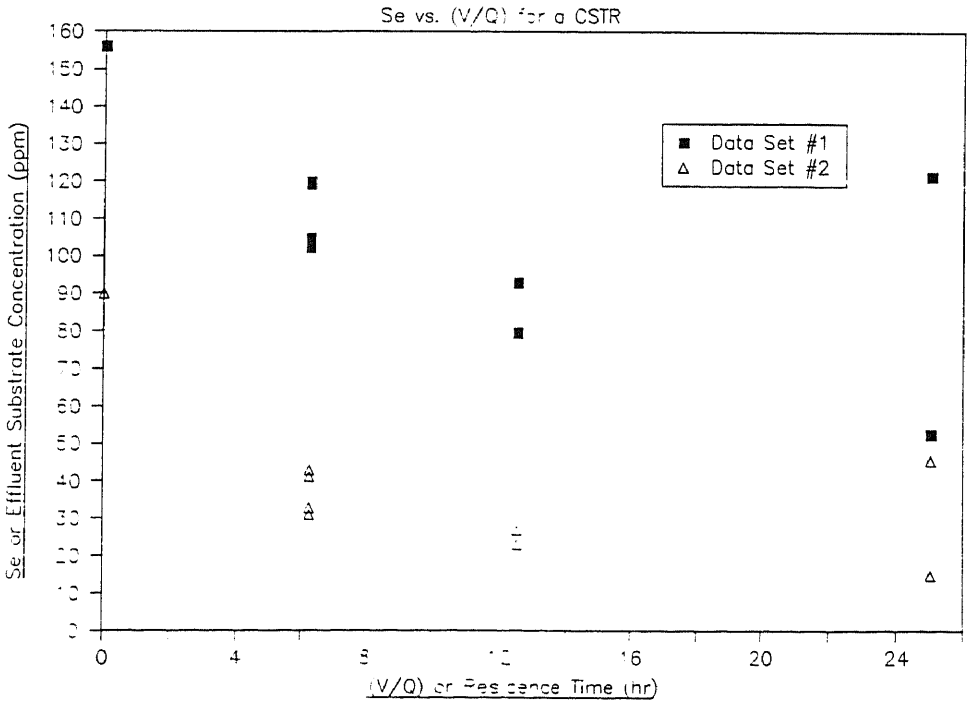
While ko is the same within experimental error for the 2 sets, K differs due to substrate-inhibitory related effects which are accounted for by the authors of this article in a model by redefining K as a linear function of Se (i.e., K = K1 + K2 * Se).

Figure 101



Source : Beltrame, P., et al (1984); data sets #1 & #2 on pages D-12..D-15

Figure 102



Source : Beltrame, P., et al (1982); data sets #1 & #2 on pages D-16..D-19

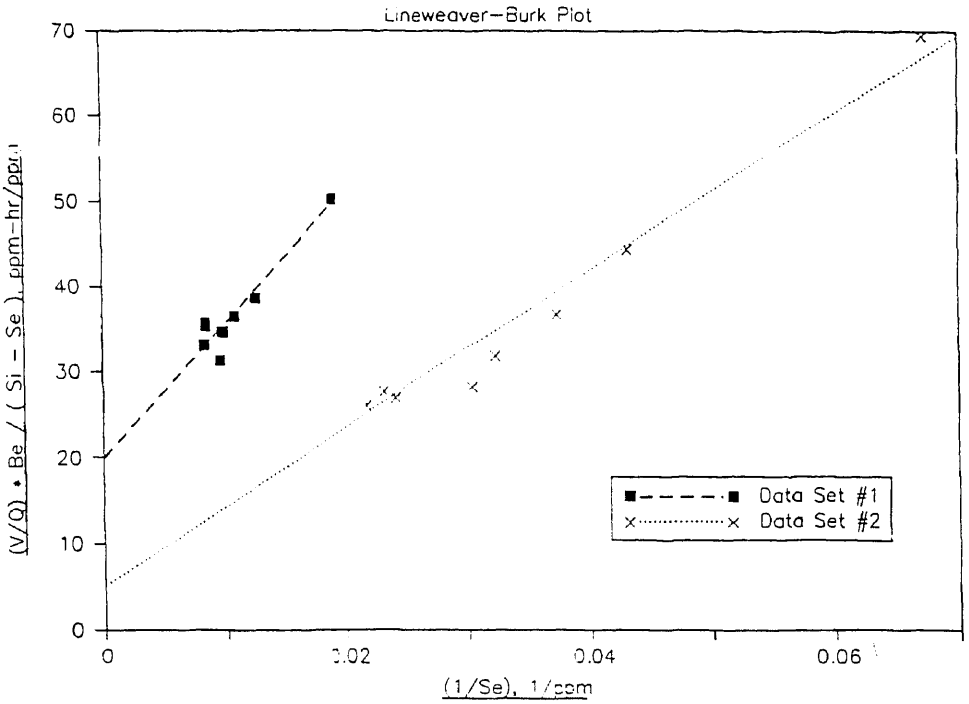
Figure 102 shows a Se vs. (V/Q) plot for 2 data sets from the other Beltrame article (i.e., from 1982) which is similar to those sets shown in Figure 99 with respect to data scatter being present due to significant variations in Be (refer to pages D-17 and D-19). Figure 103 graphically shows the corresponding Lineweaver-Burk plots for the 2 data sets to be reasonably linear. While the MV model is best for both cases, the FV model is not much worse for data set #2 (refer to page D-19). The authors used the FV model to represent data set #2 and the MV model for data set #1. The regressed results from pages D-17 and D-19 are shown below to be in fair agreement with the regressed results presented in the article.

	Results from Appendix D		Results from Article	
	ko (hr^{-1})	K (ppm)	ko (hr^{-1})	K (ppm)
Data Set #1	0.0498	77.87	0.045 ± 0.005	63 ± 12
Data Set #2	0.000933	-----	0.00098 ± 0.00002	-----

7. Analysis of the Effect of Experimental Error in Biodegradation Data on Kinetic Model Selection

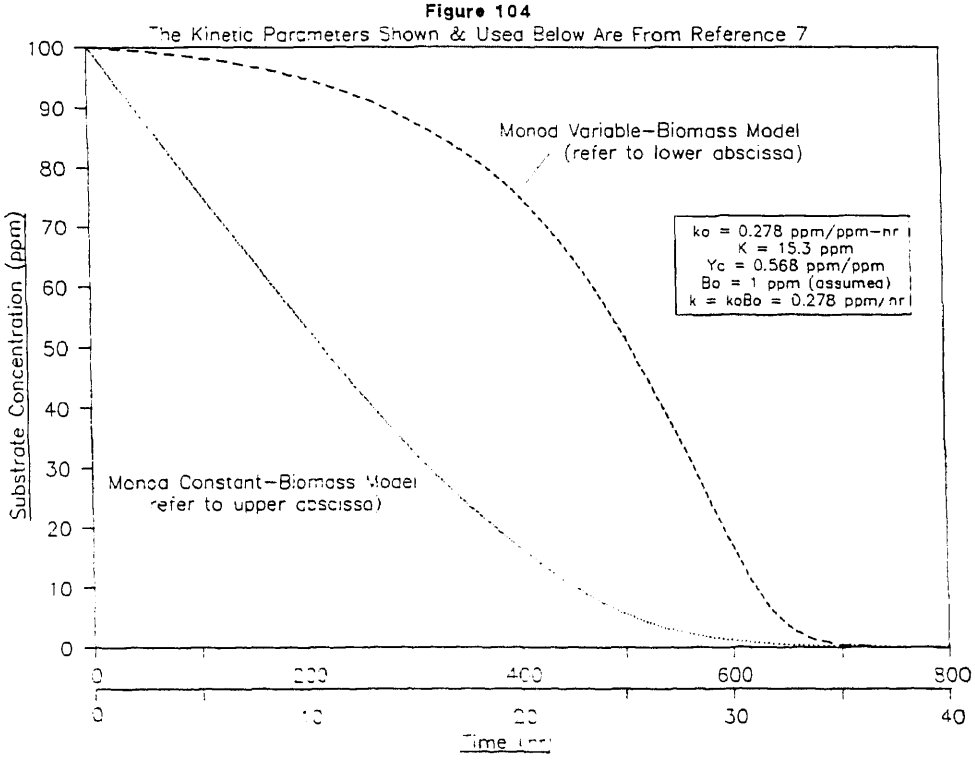
Section 6 comprehensively covered the kinetic analysis of raw aerobic biodegradation data from both batch reactors and CSTRs with respect to the constant- and variable-biomass versions of the zero-

Figure 103



Source : Beltrame, P., et al (1982); data sets #1 & #2 on pages D–16..D–19

Figure 104



order, first-order and Monod models. While the general characteristics (i.e., pros and cons) of each model for each given data type were discussed, only qualitative statements could be made as to the significance of data set quality on proper model selection. In this section, the effects of key biodegradation data measurement parameters on kinetic modelling will be systematically studied in an attempt to quantitate their impact. The ultimate goal of this effort is to establish concrete guidelines for the measurement of reliable biodegradation data for wastewater treatment reactor design purposes.

This study will be limited to the case of batch reactor data since: (1) batch reactors are commonly used for biodegradation data measurement (e.g., 140 of the 148 data sets evaluated in this thesis are from batch reactors); and (2) CSTRs have not been shown in this thesis to readily yield reliable kinetic data (refer to Section 6.3 for a description of the physical problems encountered with wall growth, imperfect mixing and achieving steady-state conditions in CSTRs). The biodegradation data measurement parameters evaluated herein in terms of their effect on proper kinetic model selection are: (1) random experimental error in S measurements, (2) number of S vs t data points, (3) data spacing/grouping, and (4) data range/truncation. While accurate measurement of biomass concentration has been repeatedly stressed within this thesis as necessary for the regression and application of the variable-biomass models, it is not assessed here because the errors in its measurement are primarily systematic (rather

than random) in nature. A discussion of the importance of accurate values of Bo and Yc (as well as the sensitivity of regression analysis to these parameters) has been covered in sufficient detail in Section 6.

7.1 Methodology

As stated previously in Section 6.1, most batch reactor data types are some variation of one of the two S vs t curves shown in Figure 1. Both of the curves can be well represented by the Monod models (i.e., M2 or M3 for Curve 1 and MV for Curve 2). As a result, the Monod models are used here as the basis for the systematic study of the effect of the experimental error and other data measurement parameters on proper kinetic model selection. It is assumed here that the "real" S vs t biodegradation data (from which abiotic mechanisms are assumed to have been excluded) are exactly as represented by the two Monod models shown in Figure 104 for the two cases of constant- and variable-biomass behavior. The kinetic parameters used as a basis for the curves presented in Figure 104 are for phenol using Pseudomonas putida and are as follows (note: Bo is assumed to be 1 ppm in both cases):[8]

$$ko = (\mu m/Yc) = (0.158/hr)/(0.568\ ppm/ppm)$$

$$= 0.278\ ppm/ppm\text{-}hr$$

$$K = 15.3\ ppm$$

$$k = koBo = (0.278\ ppm/ppm\text{-}hr)(1\ ppm) = 0.278\ ppm/hr.$$

This system was selected as the basis for this study because phenol is a commonly-encountered, well-studied substrate and Pseudomonas putida is a commonly-found culture in activated sludge with known activity toward phenol utilization. The phenol concentration range was assumed to be 0.1-100 ppm, since that would cover most applications of practical interest.

This study basically involves the following: (1) assuming the two curves in Figure 104 represent the "real" S vs t data that would be measured under ideal circumstances, (2) extracting discrete points from the two curves and adding random experimental errors to each, (3) varying the biodegradation data measurement parameters listed in Section 7, and (4) assessing their impact on the regression analysis results. The effect of each parameter on proper kinetic model selection can be assessed either graphically (i.e., by comparing the predicted vs the ideal S vs. t curves) or analytically (i.e., by either comparing the regressed rate constants vs. those of the ideal case or by using the statistic $\Sigma(t_{predicted}-t_{real})^2$). For the ideal case, the predicted S vs t curve will be identical to the "real" one, with ko and K being the same in both cases and $\Sigma(t_{predicted}-t_{real})^2$ being zero.

A brief discussion as to the manner in which the random experimental error was added to the discrete points from the "real" curves (from Figure 104) follows here prior to proceeding with a discussion of the results. First, a hundred equally spaced points (with respect to time) were extracted from each of the two curves in Figure 104 for the range of S from 100 ppm down to 0.1 ppm (refer to pages F-3 and F-4 in Appendix F for a tabulation of both of these sets). The IBM PC Basic program "Randomize" was then used to generate a hundred points at random between the range of 0 and 1 (refer to page F-5 for this tabulation). Figure 105 graphically displays the distribution of these randomly-generated numbers in bar-chart form. The sample of randomly-generated points taken is large enough (i.e., 100 points) such that the distribution is observed to be fairly equally spread over the range covered.

The randomly-generated points on page F-5 were then assumed to equal P(u) of the cumulative normal probability distribution:

$$P(u) = \int_{-\infty}^{u} (2\pi)^{-0.5} \exp(-(u')^2/2)du'; \quad (5)$$

where,

P(u) = probability (expressed in fraction form) of a sample from a normal distribution with standard deviation u' having a value of less than u.

u' = standard deviation

u = deviation from mean in standard deviation units

Figure 105

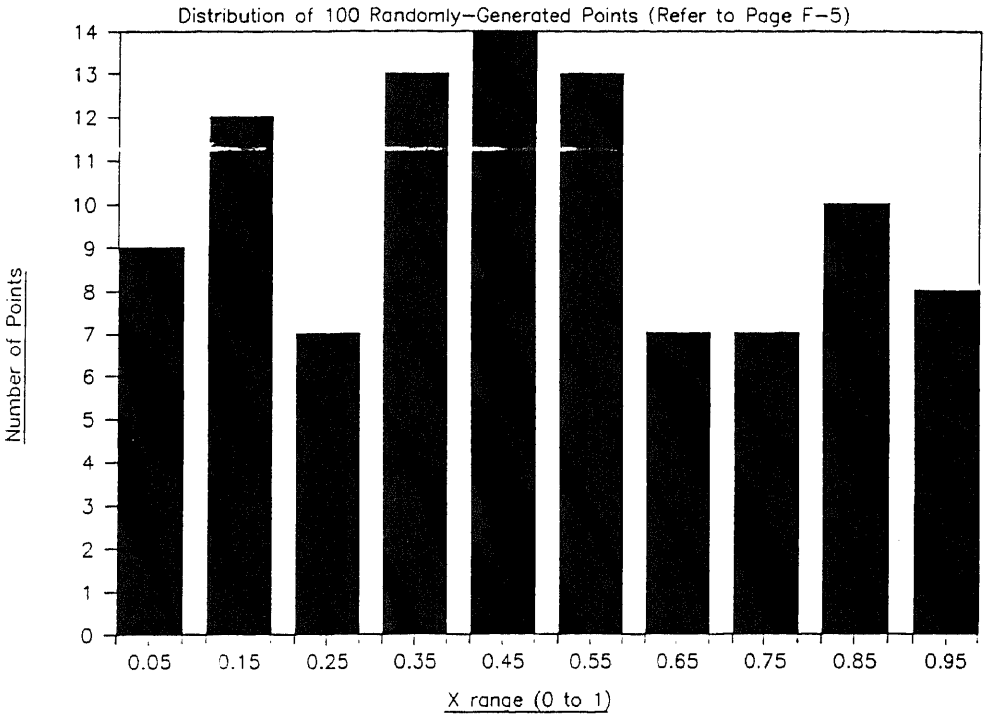
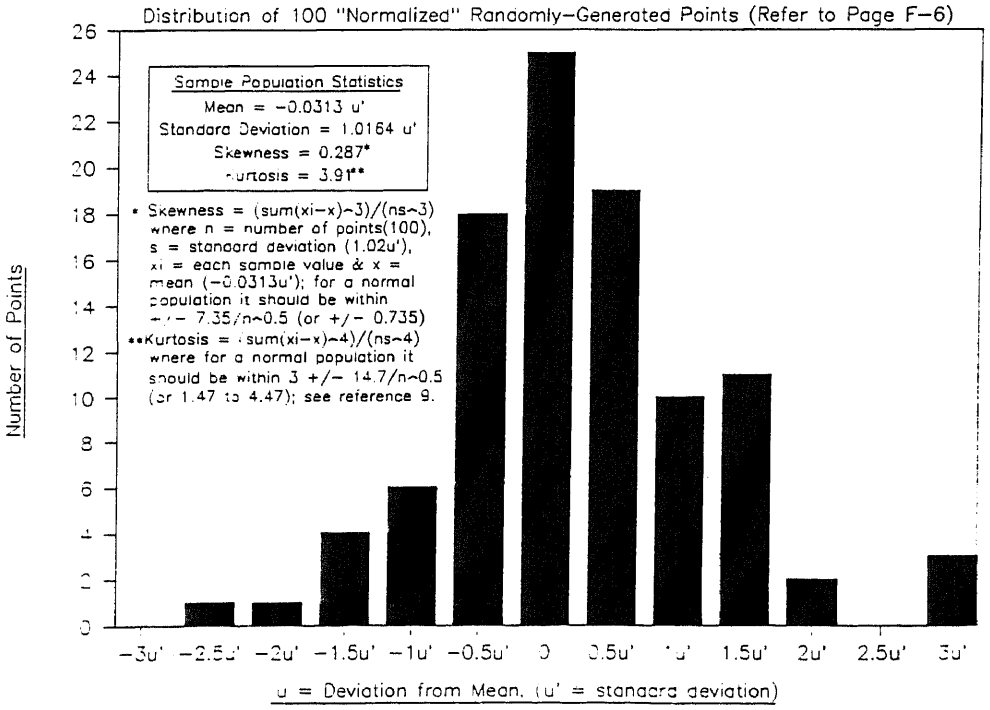


Figure 106



For each of the 100 points on page F-5, the value of u from the above expression was determined using a cumulative standard normal probability distribution table. The corresponding tabulation of u values are presented on page F-6. Figure 106 graphically presents this "normalized" random distribution in bar-chart form. The distribution of points well approximates the normal distrubition function with the calculated values of the mean and standard deviation for the sample set being close to ideal (i.e., 0 and 1 u', respectively). Furthermore, two quantitative tests prescribed by Holmes[9] (i.e., for skewness and kurtosis) to check the normality of a population were applied to the set of points from page F-5. The results (shown on Figure 106) meet the criteria established by Holmes for a normal distribution.

The above, normalized distribution was assumed in this study to represent the random error in S experienced during experimental measurement. Different levels of accuracy were assessed in this analysis by assuming different values of u'. In each case, the hypothetically measured value of S was determined by adding the value of u from page F-6 (which is first multiplied by the assumed value of u') to the corresponding "real" value of S from either pages F-3 or F-4. In this manner, the effect of random error in S was able to be studied (with respect to kinetic model performance) in a controlled fashion.

7.2 Discussion of Results

The effect of the total number of data points on regression results was evaluated for the case in which no experimental error was introduced to the two data sets on pages F-3 and F-4. For both data sets, regression analyses were performed (for the S range from 100 ppm down to 0.1 ppm) for each of the following number of equally-spaced (i.e., with respect to time) data points: (A) 100, (B) 34, (C) 12, (D) 10, and (E) 4. The results are presented on pages F-7 through F-12.

For the case in which constant-biomass behavior was assumed (i.e., the data set from page F-3), the effect of the total number of data points (down to a minimum of 4 data points) on the regression results can be seen on pages F-7 through F-9 to be insignificant for the case of "perfect" data (i.e., no experimental error present). The slight improvement in performance (in terms of $\Sigma(t\text{-}tcalc)^2$ and the regressed values of ko and K) as the number of points is reduced is due to the fact that the latter points of the set are given only to two significant figures. This introduces error into the regressed values of ko and K, which increases with the total number of points used from this latter portion of the data set.

Likewise, for the case in which variable-biomass behavior was assumed (i.e., the data set from page F-4), no significant effect of the number of data points on regression results is observed for the case of "perfect" data (i.e., $u' = 0$). The slight improvement in the performance of MV with decreasing number of data points is again attributed to the use of fewer points from the latter, less accurate, portion of the data set. It should be noted that, although no significant effect of the total number of data points on regression results is observed for "perfect" data, it is logical from a statistical perspective that improved regression results would be obtained for data containing random experimental error when the sampling population (i.e., number of data points) is increased (i.e., the more data points, the better the results). This is demonstrated later in this section.

The effect of random experimental error in S measurements was evaluated for the case of constant-biomass behavior on pages F-13 through F-15. Ten equally spaced (with respect to time) S vs. t data points spanning the S range from 100 ppm down to 0.1 ppm (from page F-3) were modified to include random experimental error using the corresponding correction terms from page F-6. The following six levels

of error were evaluated: (1) u' = 0.1 ppm, (2) u' = 0.25 ppm, (3) u'= 0.5 ppm, (4) u' = 1.0 ppm, (5) u' = 2.0 ppm, and (6) u' = 5.0 ppm. Figure 107 graphically presents the individual data points for each level of error along with the corresponding regressed M2 curves. It should be noted that the ninth data point of the set (i.e., for t = 657 hr), upon being modified to include random experimental error, resulted in negative values of S for the cases in which u' was greater than or equal to 1.0 ppm. Since negative values of S are physically impossible, and because setting S equal to zero results in indeterminate calculations for the Monod models, these negative S values were arbitrarily set to a very small value of S (i.e., 0.01 ppm).

Figure 107 shows the regressed M2 models to become progressively worse as the level of random experimental error (i.e., u') increases. For the S range of interest (i.e., 100 → 0.1 ppm), the regression results become notably worse for u' values greater than 0.25 ppm (refer to pages F-13 through F-15 for a comparison of $\Sigma(t\text{-}tcalc)^2$). It should be noted that Figure 107 only shows one of an infinite number of possible variations of random error distribution within the given data set. For consistently accurate regression results, u' should be less than the lowest absolute value

Figure 107

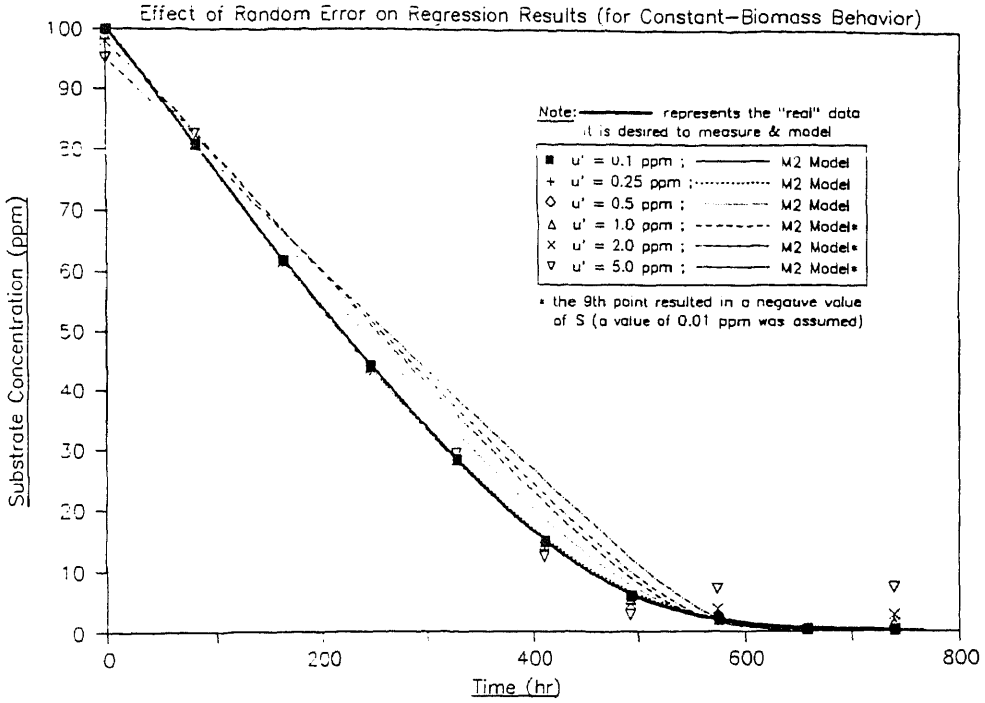
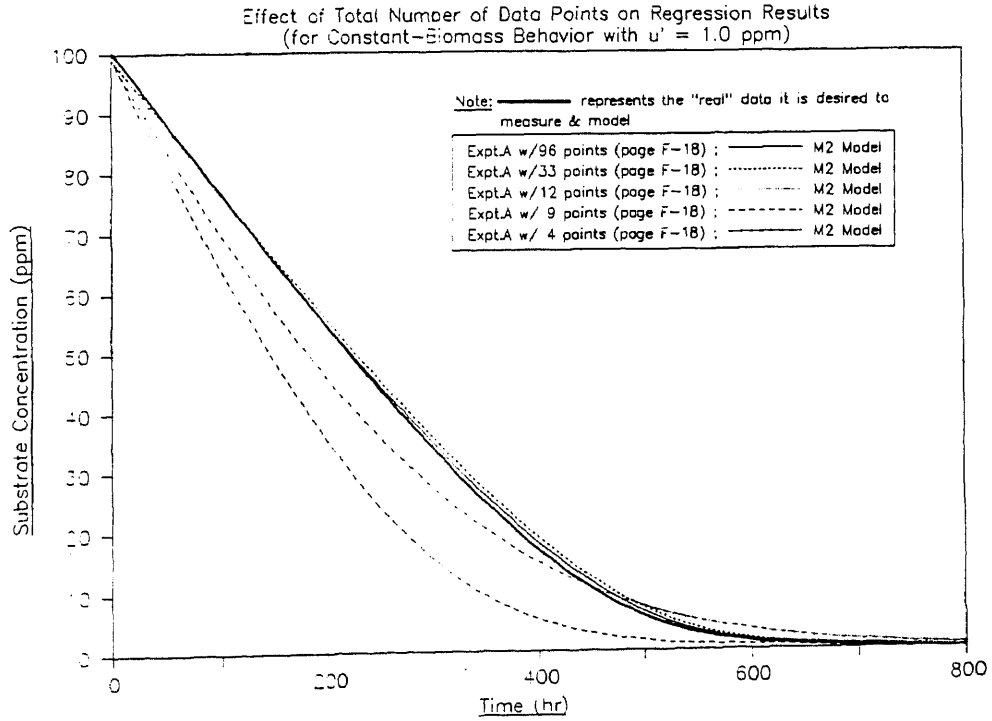


Figure 108



of S that is of interest. While increasing the number of data points will statistically result in an improvement in the accuracy of regression results for data with random experimental error (i.e., u' not equal to 0), significant errors can be expected to be introduced in the regression results for values of S lower than u'. The effect of the total number of data points on the regression results for this data set with the following two levels of experimental error is shown on page F-18: (1) u' = 1.0 ppm (refer to Figure 108), and (2) u' = 5.0 ppm (refer to Figure 109). The performance of the models, as gauged by the % error in the rate constants, improves as expected with an increase in the frequency of sampling. The statistic, $\Sigma(t\text{-}tcalc)^2$, is not as good a measure of overall performance as it only indicates the error in the measured points and not the entire curve. It should also be noted that the data points for which negative S values resulted (upon addition of the corresponding random error terms) were excluded from the analyses. This introduces systematic error into the analysis by, in effect, inflating the average S values which would otherwise be obtained in the latter portion of the curve. This is another reason why u' should be lower than the lowest value of S of interest for design purposes.

Figure 109

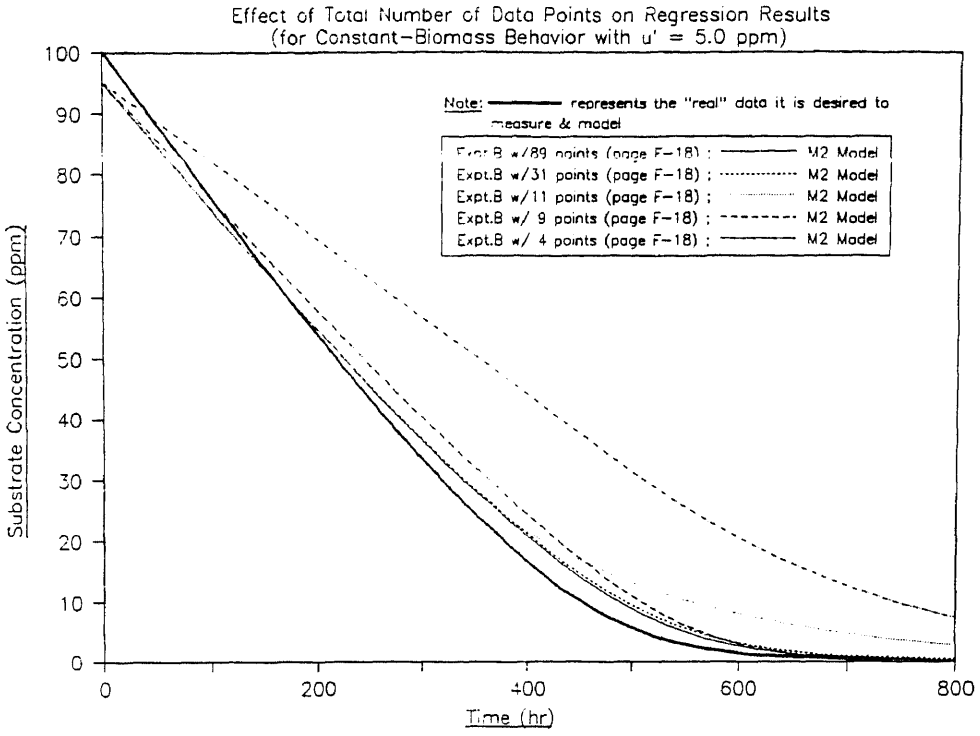
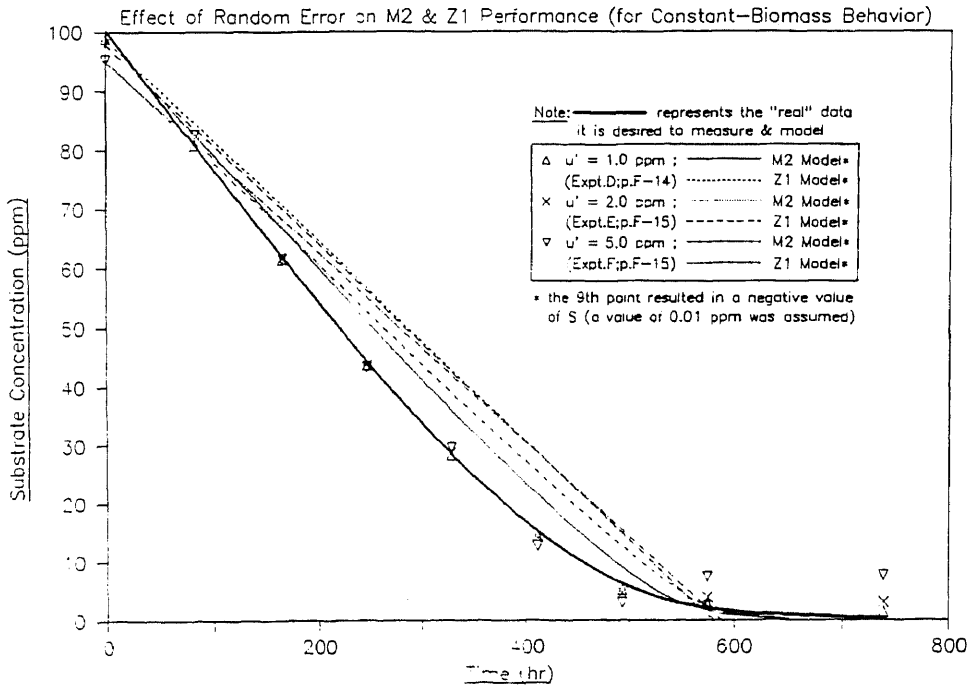


Figure 110



For the given distribution of random error in Figure 107, the constant-biomass Monod models become progressively worse as u' increases. The zero- and first-order constant-biomass models are worse (the latter much more so than the former) than the corresponding Monod models in each case, but less so on a relative basis as u' increases (refer to pages F-14 and F-15 for a tabulation of the results and to Figure 110 for a graphical presentation). The exact point at which the zero- or first-order model becomes comparable to the Monod model in performance cannot be generically predicted, but rather is a complex function of multiple parameters: (1) the system and its environment, (2) the S range covered, (3) the level of experimental error, and (4) the exact distribution of the random experimental error within the data set. For the case shown in Figure 110, the zero-order models statistically become comparable to the Monod models in performance for the case of u' equal to 5.0 ppm (note: the first-order models, however, are still much worse for this case and were, therefore, not included within Figure 110).

The effect of random experimental error in S measurements was evaluated for the case of variable-biomass behavior on pages F-16 and F-17. Ten equally spaced (with respect to time) S vs. t data points in the S range from 100 ppm down to 0.1 ppm (from page F-4) were modified to include random experimental error using the corresponding correction terms from page F-6. The same levels of experimental uncertainty were evaluated here as for the constant-biomass case.

Figure 111 graphically presents the individual data points for each level of error along with the corresponding MV curves. The performance of the MV models is seen to progressively worsen as u' increases. The MV model for error levels (i.e., u') as low as 0.1 ppm is seen to deviate from the "real" curve for values of S below 25 ppm. This deviation increases for lower values of S. Figure 111 shows that u' should be well below the lowest value of S of interest for design purposes in order to obtain accurate results for systems with strong variable-biomass effects. For values of u' equal to 2.0 ppm, the performance of the MV model in terms of $\Sigma(t-tcalc)^2$ as shown on page F-17 has deteriorated to the point that the FV and ZV models perform comparably (refer to Figure 112 for a visual comparison of the MV, ZV and FV models for this case). The constant-biomass models are notably worse than MV for each of the u' values evaluated and they are not shown here. It should be noted that regression results for the case of u' equal to 5.0 ppm are indeterminate because of negative values within ln functions. The function, f = Bo+YcSo-YcS, is negative for the second point of the set, thereby making ln (Bo+YcSo-YcS) indeterminate for that point and, hence, the entire set for each of the three variable-biomass models.

As mentioned previously for the constant-biomass case, Figure 111 presents only one of an infinite number of possible variations for the distribution of random experimental error within the data sets. In general, u' should be less than the lowest value of S that is of interest for design purposes.

Figure 111

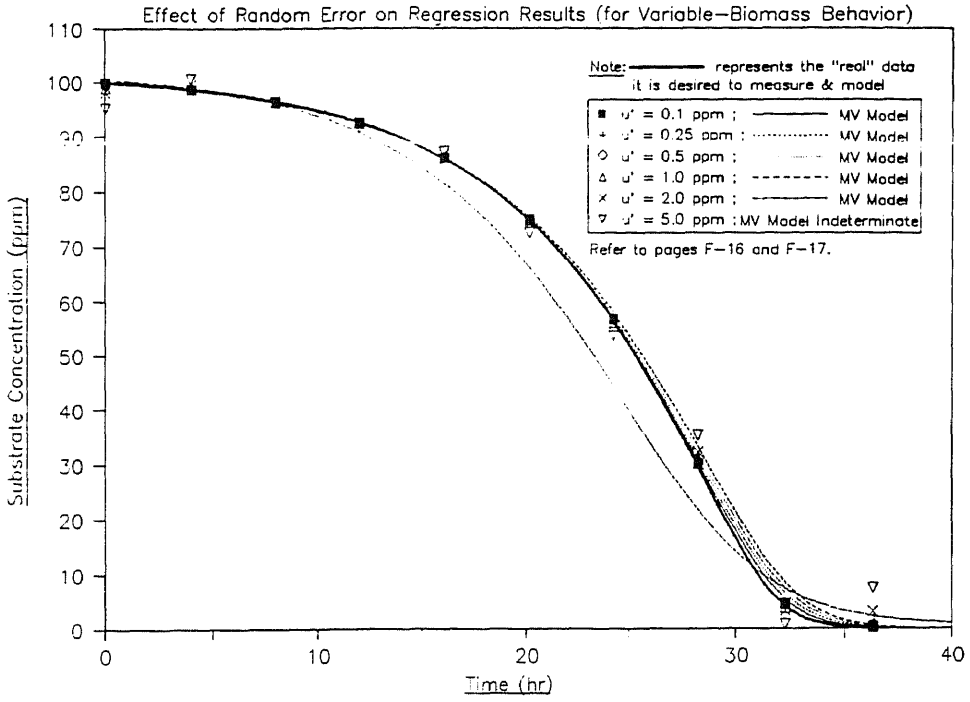
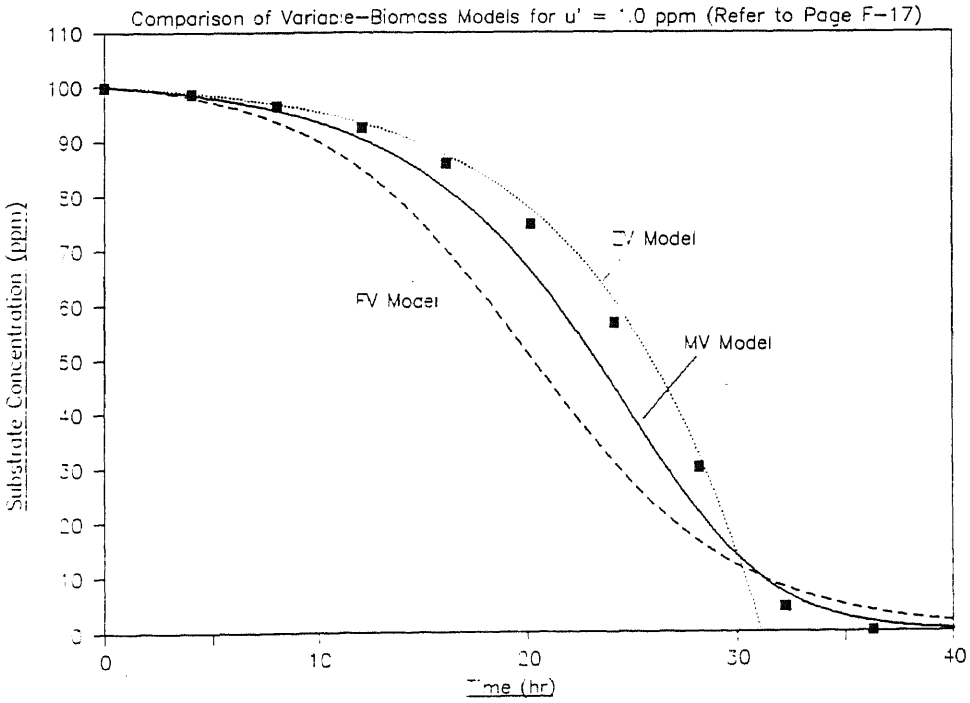


Figure 112



The effect of data spacing or regularity within a given S vs. t data set was evaluated on page F-19 for both constant- and variable-biomass kinetic behavior. Five different data spacings were assessed for each: (A) 9 points from the initial part of the set and the last point; (B) the first point and 9 points from the latter end of the set; (C) the first and last points with 8 points from the middle portion of the set; (D) 10 equally-spaced points with respect to time throughout the entire set; and (E) 10 randomly selected points from the set. In each case, a random error corresponding to a u' of 1.0 ppm was assumed (note: for the case of "perfect" data, u' = 0, no effect would be expected based on the similar finding earlier in this section for the study of the total number of equally spaced points). Figures 113 and 114 graphically present the regression results for the cases shown on page F-19. Significant variation is apparent in both figures. Whereas the distribution of random error within the given points of each case is different (thereby introducing an additional uncontrolled parameter within the study which hinders direct comparison of the results based on data spacing), it is apparent that better results (i.e., in terms of % error in ko and K) are obtained when the data are equally distributed throughout the entire range of interest. It should be noted that Case 1B (in Figure 113) and Case 2A (in Figure 114) yielded significantly different results from the other cases in their corresponding figures because the combination of random error and data spacing within each case caused least-squares analysis to regress a

Figure 113

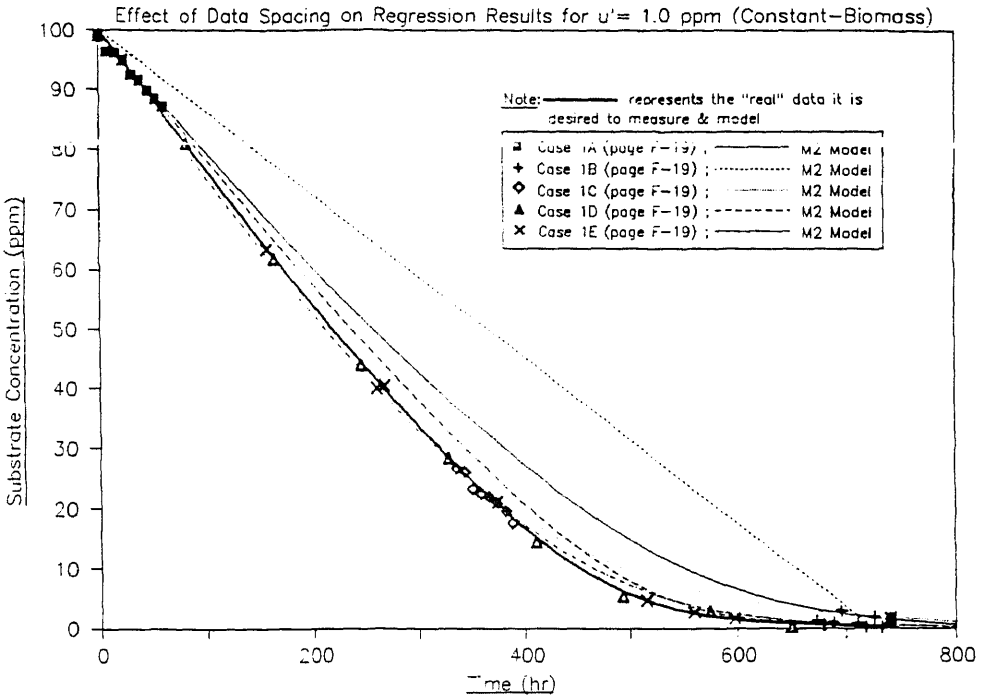
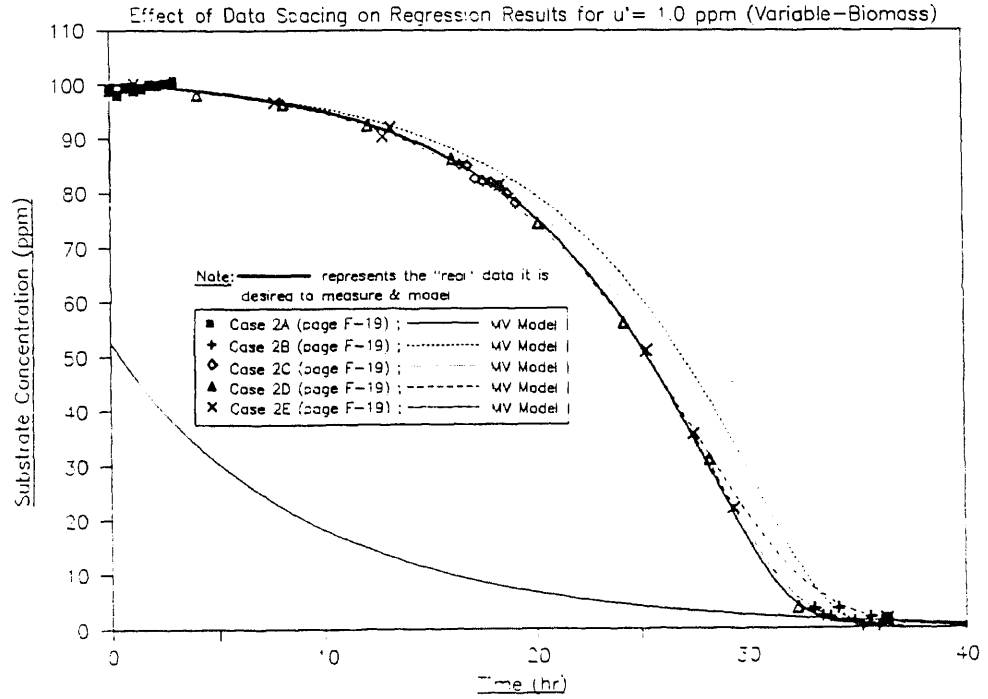


Figure 114



negative value of K and negative values of both ko and K, respectively (note: the reasons for this are discussed in detail within Section 6).

The effect of data range truncation was evaluated for the case of constant-biomass behavior on pages F-20 through F-23 (for u' = 1.0 ppm). In Experiments A through E in which the lower end of the data set is truncated progressively from 0.1 up to 25 ppm, M3 was found to be optimum (in terms of ko and K) for a lower S value of 10 ppm. At lower values of S, increased error was introduced into the regression analysis because of the higher inaccuracy of the corresponding S measurements (i.e., the ratio of u'/S increases as S decreases). At higher values of S, increased error was introduced into the regression analysis because of a reduction in the overall S range covered (i.e., the ratio of u'/(So-S) increases as S increases). Furthermore, Experiments A through E show the zero-order models to progressively improve relative to the Monod models as the lower value of S is truncated upwards. This is primarily the result of the elimination of the first-order region from the data set. Figure 115 presents a graphical comparison of the Z1 and M2 models for the S range of 100 → 25 ppm. Experiments F and G on pages F-22 and F-23 show the corresponding regression results for the S ranges from 25 ppm down to 0.1 ppm and 1.0 ppm, respectively. Both of these ranges cover the region where the transition to first-order kinetics is observed to occur. In both cases, the zero- and first-order models are statistically only a little worse than the Monod models because of the relatively large error in the data (i.e., both u'/S and u'/(So-S) are high). With more accurate data (i.e., lower values of u'), the

Figure 115

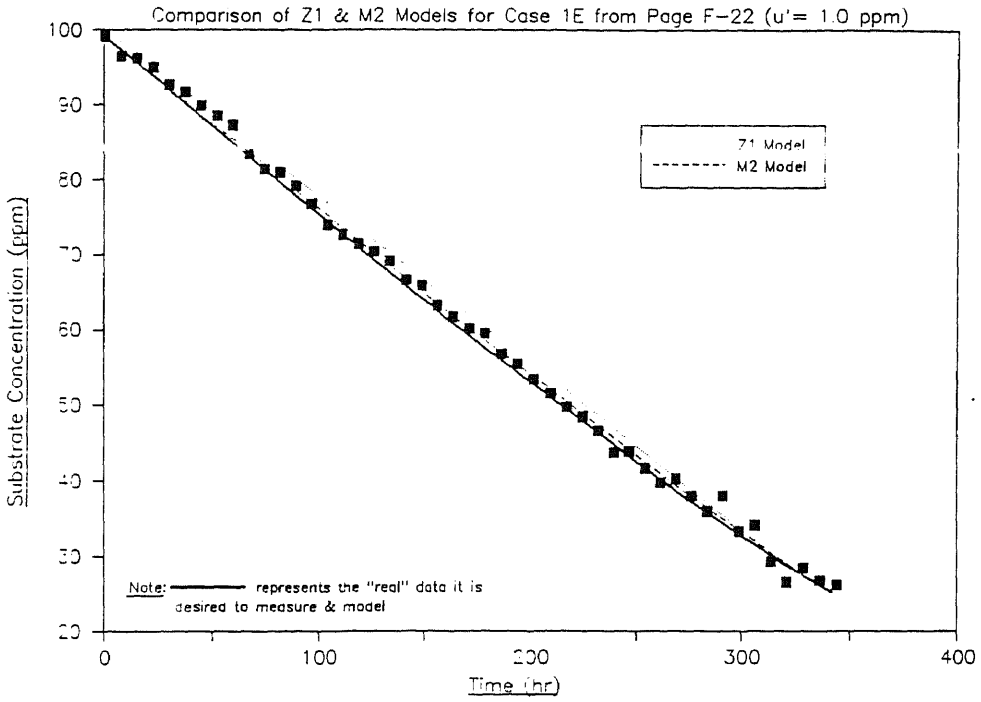
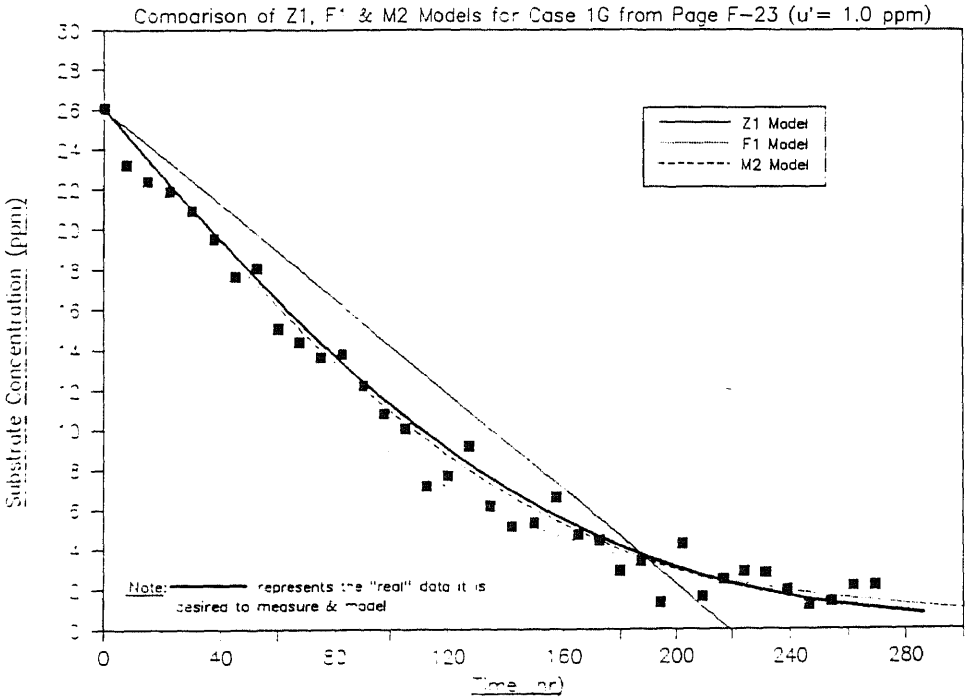


Figure 116



first-order models would be observed to perform much better than the zero-order models for the 25 → 0.1 ppm S range. Figure 116 presents a graphical comparison of the M2, F1 and Z1 models for the 25 → 1 ppm range.

The effect of data range truncation was evaluated for the case of variable-biomass behavior (for u' = 1.0 ppm) on pages F-23 through F-25 in Experiments A through E. The MV model was found to be optimum (in terms of ko and K) for the S range of 100 ppm down to 1 ppm. For lower and higher final values of S, increased error was introduced into the regression analyses for the same reasons as mentioned above for the constant-biomass case. As the S range is truncated, both the ZV and FV models improve relative to the MV model. The ZV model is the better of the two because of the exclusion of the first-order effect in the data as the S range is truncated (note: the transition from zero- to first-order kinetics occurs in the 20-40 ppm range for this case). Statistically, the FV model improves relative to the MV and ZV models as the S range is truncated because of a relative decrease in the overall accuracy of the data set as reflected by an increase in u'/(So-S). Figure 117 presents a graphical comparison of the MV, FV and ZV models for the 100 → 25 ppm range.

Regression analysis of the 25 ppm → 0.1 ppm S range for the variable-biomass case was performed for all of the constant- and variable-biomass models on page F-25 in Experiment F. In general, the Monod models are best, followed by the first-order models, with the zero-order models being worst because of the data in this case being

Figure 117

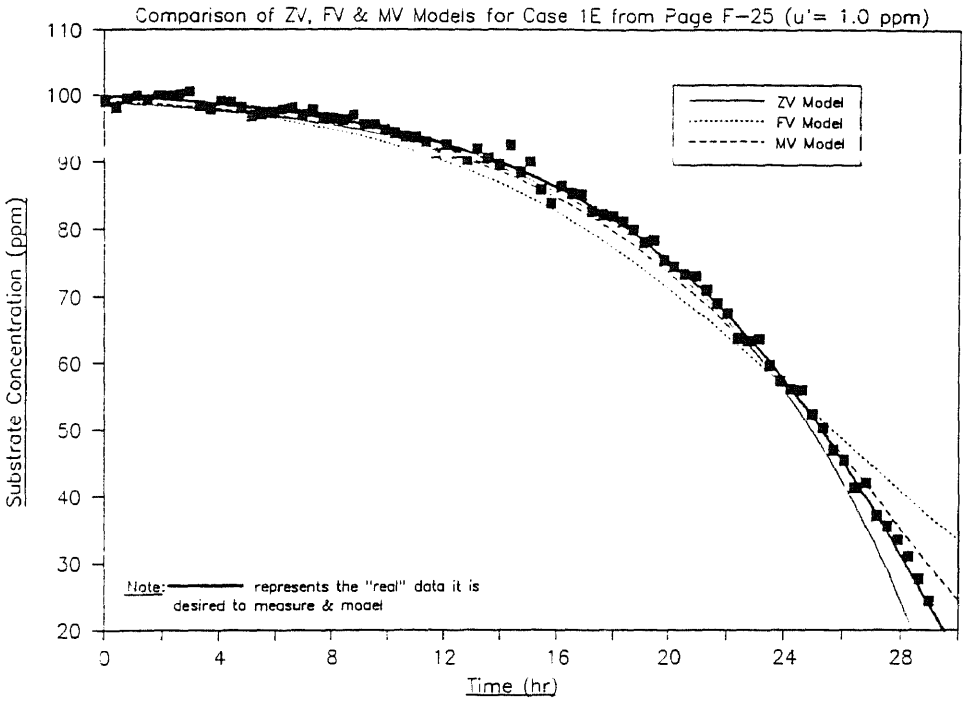
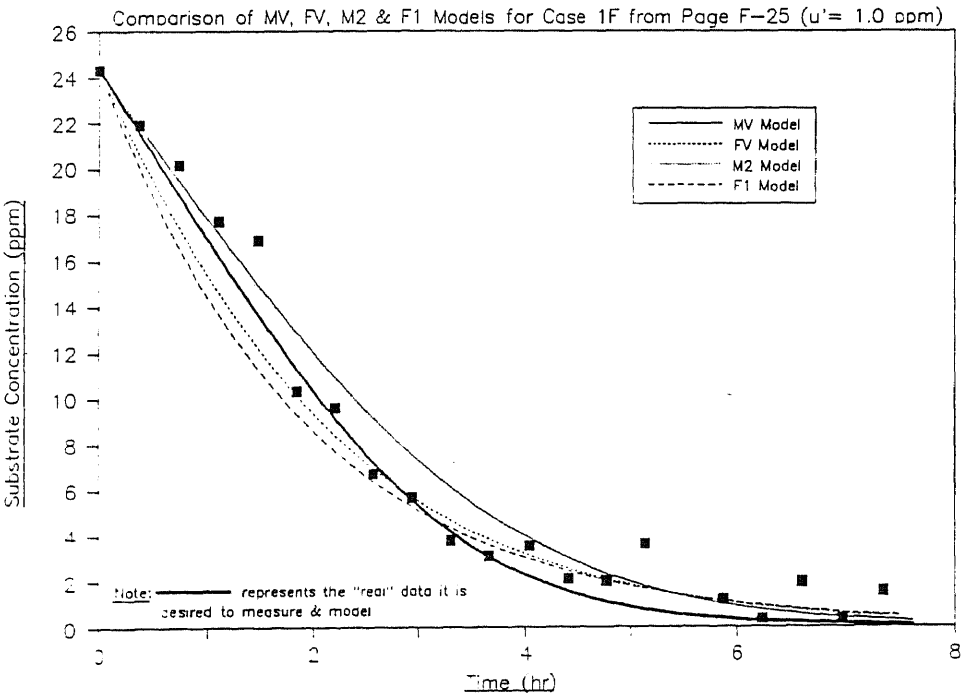


Figure 118



primarily in the first-order region. The constant- and variable-biomass models yield comparable results because the observed variable-biomass effect is relatively small (i.e., B increases only by 32% for the S range covered). Figure 118 presents a graphical comparison of the MV, FV, M2 and F1 models for this case. While all four models are comparable for the data shown (i.e., the points which include random experimental error of magnitude u' = 1.0 ppm), they all underpredict the extent of conversion relative to the "real" curve for S values below 4 ppm. This is attributed to the fact that the data points in the latter portion of the curve are, on average, higher than the "real" points because of exclusion from the regression analysis of S values equal to or less than zero. Use of arbitrarily low positive values of S (e.g., S equal to 0.01 ppm) in place of the excluded values improves the regression results slightly, but the average value of S in the latter portion of the curve will still be higher than the "real" values as a result of the arbitrary increase in some of the randomly measured S values. This is a real concern whenever data measurements are made for S values of magnitude less than 3 u'.

8. Potential Benefits from Proper Model Selection

The potential benefits from proper model selection lie in the sizing of wastewater treatment reactors. An accurate model will result in the minimum reactor volume that meets design objectives. An inaccurate model will result in an inefficient design in which the reactor will either be oversized (thereby increasing capital cost) or

undersized (thereby not meeting pre-determined specifications for throughput and/or removal efficiency). The extent of oversizing or undersizing can readily be quantitated in terms of the ratio of the predicted reactor volume, Vp, to that of the theoretically minimum reactor volume, Vt, necessary to meet pre-established specifications. The ratio Vp/Vt for a CSTR is equal to the ratio of the theoretical reaction rate, (-rt), to the predicted reaction rate, (-rp). Values of Vp/Vt greater than 1 indicate oversizing while values less than 1 indicate undersizing.

A summary of analytical expressions for Vp/Vt are provided in Table 6 for a CSTR. Each expression shown refers to the volumetric inefficiency in CSTR sizing which results from the use of the indicated model instead of the theoretical or "real" model it is desired to determine. For the expressions shown, the theoretical or "real" model is assumed to be a Monod model (either M2/M3 for the case of constant-biomass behavior or MV for the case of variable-biomass behavior) with kinetic constants designated with asterisks. Examples of the effect of incorrect or inaccurate model selection on volumetric efficiency (i.e., Vp/Vt) in reactor design for selected cases from Section 7.2 are presented below.

Table 6

Summary of Vp/Vt Expressions for a CSTR for the Cases of Constant- and Variable-Biomass Behavior[1]

Constant-Biomass Behavior:

Z1/Z2 Model: (Vp/Vt) = (k*Se)/(k(K*+Se))

F1/F2 Model: (Vp/Vt) = k*/(k(K*+Se))

M2/M3 Model: (Vp/Vt) = (k*(K+Se))/(k(K*+Se))

Variable-Biomass Behavior:

ZV Model: (Vp/Vt) = (ko*Se)/(ko(K*+Se))

FV Model: (Vp/Vt) = ko*/(ko(K*+Se))

MV Model: (Vp/Vt) = (ko*(K+Se))/(ko(K*+Se))

Z1/Z2 Model: (Vp/Vt) = (ko*(Bi+Yc(Si-Se))Se)/(k(K*+Se))

F1/F2 Model: (Vp/Vt) = (ko*(Bi+Yc(Si-Se)))/(k(K*+Se))

M2/M3 Model: (Vp/Vt) = (ko*(Bi+Yc(Si-Se))(K+Se))/(k(K*+Se))

1 The Vp/Vt expressions shown refer to the volumetric inefficiency in reactor sizing resulting from the use of the indicated model in place of the theoretical or "real" model it is desired to determine. The theoretical or "real" model is assumed to be a Monod model (M2/M3 for constant-biomass behavior or MV for variable-biomass behavior) with the kinetic constants designated by the asterisks.

The effect of incorrect model selection on CSTR design for the case of ideal constant-biomass behavior (i.e., u'=0) is demonstrated as follows in terms of Vp/Vt for the regressed models from Experiment D on page F-8 for CSTRs with Se values of 0.1 ppm:

Model	Vp/Vt
M3	1.000
M2	1.000
Z2	0.012
Z1	0.010
F2	1.804
F1	2.329

The Monod models, as expected for ideal data with no experimental error, yield perfect results in terms of Vp/Vt. Use of the above incorrect zero-order models for CSTR design would result in significantly undersized vessels. The desired conversion of substrate in these vessels could only be achieved at dramatically reduced throughputs (i.e., ca. 1% of design). The above incorrect first-order models, unlike the zero-order models, result in oversized vessels. While these vessels would achieve the pre-established design specifications, it would be accomplished at a much higher capital investment than necessary. For the case of ideal constant-biomass data intermediate in order between zero and first, the zero-order models will always result in undersized vessels (ie., Vp/Vt <1) while the first-order models will always result in oversized vessels (i.e., Vp/Vt >1).

The corresponding effect of incorrect model selection on CSTR design for the case of ideal variable-biomass behavior (i.e., u'=0) is demonstrated as follows in terms of Vp/Vt for the regressed models from Experiment D on page F-11 for CSTRs with Se values of 0.1 ppm:

Model	Vp/Vt
MV	1.000
M3	-0.799
M2	-2.169
ZV	0.008
Z2	0.031
Z1	0.041
FV	4.520
F2	4.363
F1	7.189

As for the case of ideal constant-biomass data, all of the zero-order models underpredict Vt, while all of the first-order models overpredict Vt, for kinetic data of fractional order. The above M3/M2 models yield physically uninterpretable results for Vt because the regressed models from page F-11 had negative values of K. The negative values of Vp/Vt result above because the value of Se selected (i.e., 0.1 ppm) is less than the absolute values of K in both cases.

The effect of inaccuracy in regressed constants, resulting from random experimental error (i.e., u' not equal to 0), for theoretically correct models on CSTR sizing is presented below for the cases of constant- and variable-biomass behavior from pages F-13 through F-15 and from pages F-16 and F-17, respectively:

Experiment	u'(ppm)	Vp/Vt for M3 (p. F-13 to F-15)	Vp/Vt for MV (p. F-16 and F-17)
-	0	1.000	1.000
A	0.1	1.109	1.153
B	0.25	1.073	1.255
C	0.5	0.701	1.327
D	1.0	0.435	1.373
E	2.0	0.371	2.747
F	5.0	0.253	N/A

The above results demonstrate the importance of minimizing experimental error (i.e, u') in raw kinetic data in terms of obtaining models which accurately depict reality and result in effective and cost-efficient wastewater treatment reactor designs. It should be noted that the above trends in Vp/Vt with respect to u' for both M3 and MV are the result of the particular distribution of random error evaluated in Appendix F and not any inherent characteristics of the models.

The effect of inaccuracy in regressed constants from theoretically correct models, resulting from different data sampling spacings/regularity for the case of u' equal to 1.0 ppm, on CSTR sizing is presented below for the cases of constant- and variable-biomass behavior shown previously in Figures 113 and 114, respectively:

Case	Description	Vp/Vt for M2 (refer to Fig. 113)	Vp/Vt for MV (refer to Fig. 114)
A	Mostly initial points	1.517	10.924
B	Mostly final points	-0.015	0.750
C	Mostly central points	2.227	1.603
D	Equally spaced points	0.902	1.152
E	Randomly spaced points	1.439	1.844

The above tabulation clearly demonstrates that the best results are obtained when sampling is performed on a regular basis with respect to time over the entire S range of interest. Highly erroneous results can be obtained when sampling is concentrated over a time interval short enough such that u' is greater than the actual substrate converted, as demonstrated above in cases A and B. Case B for M2 and Case A for MV are especially bad because of the regression of negative rate constants for reasons stated previously in Section 7.2.

The effect of inaccuracy is regressed constants, resulting from random experimental error in S (i.e., u') which approaches the absolute magnitude of S, on CSTR sizing is presented below for the models and case shown previously in Figure 118:

Model	Vp/Vt
MV	1.250
FV	1.826
M2	1.272
F1	2.096

Each of the above regressed models resulted in oversizing of CSTRs because of inherent systematic error in the S data in the range where S is less than 3u'. In this S range, the average value of S is inflated because of the exclusion of negative values of S which would naturally occur if the physical lower limit of 0 were not present. Whereas arbitrarily low positive values of S were used in place of S values less than or equal to 0 for the hypothetical cases evaluated in Section 7, this approach only alleviated the problem partially by lowering the average S value for the latter part of the range slightly (i.e., vs. what the average would have been if these values had been excluded entirely). Since the values which would otherwise be negative were arbitrarily increased to positive values, the average "measured" S value is naturally higher than the "real" S values it is desired to measure. The above example further demonstrates the need for controlling u' below one third of the lowest value of S of interest for design purposes in order not to regress models which result in oversized vessels.

9. Conclusions

Review of the open literature has demonstrated that a significant inconsistency exists with respect to the selection of kinetic expressions by authors for the modelling of raw aerobic biodegradation data. A total of 140 batch reactor biodegradation data sets extracted from the literature and previous NJIT MS theses were categorized, according to the shapes of the S vs. t curves, within the following nine biodegradation data types: (1) zero-order constant biomass, (2) first-order constant biomass, (3) Monod constant biomass, (4) Monod variable biomass, (5) first-order variable biomass, (6) zero-order variable biomass, (7) lag followed by biodegradation, (8) greater than first order, and (9) miscellaneous.

The latter two data types have no theoretical bases within biodegradation kinetics and refer to observed S vs. t curves which are more likely artifacts of the experimental methods used than intrinsic kinetic data. The common causes of data types 8 and 9 were: (i) failure to eliminate abiotic substrate removal mechanisms (e.g., adsorption, evaporation, etc.), and (ii) poor quality data (i.e., insufficient/inaccurate measurements).

The first seven data types are typical of batch reactor aerobic biodegradation data where abiotic mechanisms have been removed and mass-transfer resistances are not limiting. Furthermore, each of the first seven data types can be observed to be derived from either one or both of the two generalized biodegradation curves presented in Figure 1. While variations of the Monod model appear to be the preferred method of data analysis in most cases, this model suffers from certain problems in specific instances which hinder its universal application. Model selection recommendations given here, therefore, vary with data type. The initial critical step in the model selection procedure is the categorization of a given data set within one of the above-mentioned data types based on the shape of its S vs. t curve.

For type 1 data, the constant-biomass Monod model always yields statistically better results than the corresponding zero-order model because of the additional degree of freedom in the regression analysis provided in the Monod model by the kinetic parameter K. The Monod model, however, will regress negative values of K for type 1 data whenever the S vs. t curve can be interpreted as bending downward

(possibly as a result of random experimental error). The zero-order model is generally preferred for type 1 data, but only for application over the range of S data evaluated, since extrapolation errors can be very large.

For type 2 data, the constant-biomass Monod model will always yield statistically better results than the corresponding first-order model because of the inherent additional regressable parameter K. The Monod model, however, will regress negative values of both k and K for type 2 data whenever the S vs. t curve can be interpreted as dropping at a rate any greater than first order (possibly as a result of random experimental error). In general, the first-order model is preferred for type 2 data. It should also be noted that So should always be treated as a regressable parameter since it results in statistically better fits than when it is set equal to the initial substrate concentration. In this way, a given model can average out random experimental error over **all** of the data points in a given set, thereby eliminating any bias toward the first data point of a set which occurs when So is arbitrarily set equal to S at t=0. The logic behind the regression of So is that, if So is measured in the same way as any other value of S (e.g., by GC analysis which is the case in the data from previous NJIT MS theses), then it has no claim to an exact value.

Type 3 data are the most common for batch reactor aerobic biodegradations utilizing substrate-acclimated cultures of virtually constant biomass concentration. These data sets are of fractional order (i.e., intermediate between zero and first) and are very well represented by the constant-biomass Monod model.

The variable-biomass models reduce to the corresponding constant-biomass versions for data types 1 through 3, thereby yielding identical results in the above cases. It should be noted that the prediction of whether a given system prior to measurement will be of types 1, 2 or 3 cannot be reliably made based on knowledge of the substrate concentration range covered alone. The kinetics are determined primarily by the S/B (i.e., substrate to active biomass concentration) ratio, as well as a host of other complex environmental and metabolic factors. Determination of the S/B ratio alone is difficult due to the lack of a simple procedure by which to measure the active biomass concentration, B, accurately.

While the active biomass concentration is never truly constant due to the incessantly changing conditions within the reactor environment, data types 4 through 6 specifically refer to systems in which the active biomass concentration changes (i.e., increases) many-fold over the range of S utilized. Since biomass yield coefficients, Yc, are low (i.e., typically between 0 and 1), the many-fold increase mentioned above will only be observed in cases where the initial active biomass concentration, B_o, is low. The main problem observed in this

thesis, for the cases where strong variable-biomass effects were evident, is that of accurately measuring Bo. All of the authors studied herein measured the total (not active) biomass concentration which did not vary proportionately with the active biomass concentration. The biomass determination methods used (e.g., dry biomass weight and absorbance) do not differentiate between substrate-specific and non-substrate specific cultures, let alone between living and dead cells of the substrate-specific culture(s). Reasonable regression results were only obtained herein for single culture (as opposed to the more common mixed culture) systems. Whereas the variable-biomass effects were still underpredicted due to overestimation of Bo because of the inability of the above methods to differentiate between living and dead cells, Bo was much less overestimated than in the mixed culture systems where non-substrate-specific cultures provided additional interferences.

The variable-biomass Monod model, MV, yields statistically better results than both the zero- and first-order variable-biomass models for all batch reactor data of types 4 through 6. While the MV model is relatively insensitive (i.e., compared to ZV and FV) to inaccuracies in biomass measurement in terms of fit (i.e., $\Sigma(t\text{-}tcalc)^2$), it is very dependent on accurate B values with respect to regressing positive values for the rate constants ko and K. MV will regress negative values of K if the value of Bo is sufficiently overestimated and it will regress negative values of both ko and K if

Bo is sufficiently underestimated. While the FV model yields positive rate constants for all values of Bo and has similar characteristics (i.e., in terms of curvature) to that of the MV model, the adequacy of fit in terms of $\Sigma(t\text{-}tcalc)^2$ is critically dependent on accurate Bo values. The conclusion here is that the MV model is best for data of types 4 through 6, but it requires more accurate measurement of active biomass concentration than is typically being accomplished in the literature.

Biodegradation data type 7 can be reasonably well fit by the variable-biomass models for the cases where: (i) accurate active biomass measurements are available, (ii) the lag is relatively short compared to the overall biodegradation time, and (iii) the transition from lag to biodegradation is gradual and not abrupt. The above conditions are not always met and better regression results are obtained by excluding the lag from the analysis entirely. This is the recommended approach until a better theoretical model, depicting the metabolic activities associated with the lag phase, is developed.

While many of the batch reactor aerobic biodegradation data sets evaluated in this thesis could be well represented by kinetic models, the applicability of the resulting models is limited by inadequate description of the biomass system. This limitation was demonstrated in this thesis by the regression of significantly different rate constants for purportedly identical reaction systems/conditions.

For a given model to be useful, it is necessary to know the exact conditions under which the data on which it is based was determined. Specifically, the types and concentrations of substrate-specific cultures must be known, as well as the interactive relationships between cultures and the effect of changes in the environment on their performance, in order for a given data set to be of general use for design purposes. This point cannot be underestimated. The biomass is a catalyst and needs to be defined as well as any catalyst for synthetic purposes in order for the data derived from it to be useful. This is the area where the literature and current technology is most lacking.

8 CSTR aerobic biodegradation data sets were also extracted from literature and kinetic analyses were performed on them. The quality of the data from CSTRs for modelling purposes was found to be much worse than that from batch reactors primarily due to problems associated with wall growth and the inability to readily achieve steady-state conditions. Other factors found to hinder the quality of CSTR data were: (i) most measurements were made at residence times so high that virtually complete conversion was achieved; the resulting Se values, therefore, had relatively high experimental errors associated with them; and (ii) most of the data were for CSTRs with controlled sludging which caused the regression results to rely too heavily on

relatively inaccurate point measurements of active biomass concentration. For kinetic analysis purposes, CSTR operation as a chemostat with measurements at shorter residence times, where lower conversions occur, is recommended.

Significant variation in data quality was observed, in terms of analytical accuracy, sampling regularity and frequency, for the 148 data sets studied in this thesis. A theoretical analysis of the effect of data quality (i.e., specifically with respect to substrate concentration measurements) on regression results was, therefore, conducted for the cases of ideal constant- and variable-biomass batch reactor aerobic biodegradation data sets in order to establish some general guidelines in this area. For the case of **ideal** data (i.e., with no experimental error), no effect on the regression of rate constants for the theoretically correct Monod models is observed with variation in sampling frequency, regularity and range, providing a minimum of 4 data points exist. As random experimental error is introduced into the data sets, however, better regression results are obtained by maintaining sampling regularity and increasing sampling frequency. Random experimental error (as measured in terms of the standard deviation, u') should be such that u' is less than one third of the lowest value of S it is desired to measure. Otherwise, a systematic error will be introduced into the regression analysis due to the data points, on average, in the latter portion of the set where S is less than 3 u', being higher than reality because of the physical

impossibility of measuring negative values of S. Small errors in the latter portion of the set have a greater impact on the accuracy of regression results for the Monod model than comparable errors in other portions of the set because of the logarithmic functions in the linear regression analyses which inherently favor the lower values of S in terms of fit. With respect to the effects of sampling frequency, regularity and range, as well as analytical accuracy, on the fit of incorrect models (e.g., zero and first order), the only general observation that can be made is that differentiation between all models (i.e., theoretically correct and incorrect models) decreases as data quality worsens. No generalization can be made with respect to at which point the incorrect models become comparable to the correct models as a result of experimental measurement errors.

Accurate kinetic models are of importance for wastewater treatment reactor sizing. For typical biodegradation kinetics which are of fractional order, zero-order models will underpredict reactor volume (thereby failing to meet pre-established specifications for throughput and/or removal efficiency) while first-order models will overpredict reactor volume (thereby increasing the capital cost required to meet pre-established specifications). Reactor sizing, for the cases in which theoretically correct models are used, is sensitive to errors in the rate constants resulting from random experimental

error in substrate concentration measurements. Random error should be such that u' is less than one third of the lowest value of S it is desired to measure in order to yield a reliable, cost-efficient reactor design.

10. References

1. Monod, J. (1949). The Growth of Bacterial Cultures. Annual Reviews of Microbiology, 3, 371-394.

2. Pike, E. B. and E. G. Carrington (1972). Recent developments in the study of bacteria in the activated-sludge process. Water Pollution Control, 71, 583-605.

3. Pirt, S. J. (1965), Proc. Royal Soc. Ser. B, 163, 224.

4. Yang, R. D. and A. E. Humphrey (1975). Dynamic and steady state studies of phenol biodegradation in pure and mixed cultures. Biotechnol. Bioeng., 17, 1211-1235.

5. Yoon, H. G., Klinzing and H. W. Blanch (1977). Biotechnol. Bioeng., 19, 1193.

6. Grau, P. and M. Dohanyos (1971). Kinetic assessment of glucose removal and saccharide accumulation capacities in activated sludge. Proceedings of the 5th Int'l. Conf. on Water Pollution Res., Paper NoII-3, San Francisco.

7. Carberry, J. (1976). Chemical and Catalytic Reaction Engineering. McGraw-Hill, Inc., 82.

8. Lewandowski, G. A., B. C. Baltzis, C. -M. Kung and M. E. Frank n1988). An approach to biocatalyst modelling of mixed population using pure culture kinetic data. Biotechnology Applications in Hazardous Waste Treatment, Engineering Foundation, Longboat Key, Florida.

9. Holmes, D. (1988). Introduction to SPC. Stochos, Inc., 11-16.

Appendix A

Mathematical Derivation of Kinetic Expressions for the Regression of Biodegradation Rate Constants from Batch Reactor Data

Table of Contents

Nomenclature

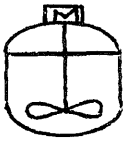
a,b,c = regressable parameters

A1, A2, A3
B1, B2, B3
C1, C2, C3
D1, D2, D3
E1, E2, E3
F1, F2, F3
G1, G2, G3
H1, H2, H3
I1, I2, I3

= variables used in matrix calculations (as defined on A-20 to A-22)

B = biomass concentration = Bo + Yc (So-S)
Bo = initial biomass concentration
k = biodegradation rate constant = koB
K = constant for Monod kinetic expression
ko = biodegradation rate constant (independent of biomass concentration)
n = number of data points
r = biodegradation rate (ppm/hr)
S = substrate concentration (ppm)
So = initial substrate concentration (ppm)
t = time elapsed (hr)
x, y, z = variables used in regression analyses
Y = variable used in regression analyses
Yc = yield coefficient = (B-Bo)/(So-S)

Ideal Batch Reactor:(Performance Equation)



assume:

i. uniform composition throughout reactor

ii. constant reactor volume

mass balance: ~~input~~ = ~~output~~ + disappearance + accumulation

$\therefore$ disappearance = -accumulation

$$\begin{bmatrix}\text{rate of loss of substrate}\\ \text{within reactor due to}\\ \text{chemical reaction}\end{bmatrix} = -\begin{bmatrix}\text{rate of accumulation}\\ \text{of substrate}\\ \text{within the reactor}\end{bmatrix}$$

$$(-r) = -dS/dt$$

$$dt = -dS/(-r)$$

$$\int_0^t dt = -\int_{S_o}^{S} dS/(-r)$$

therefore, $\boxed{t = -\int_{S_o}^{S} dS/(-r)}$; performance equation

Zero-Order Kinetics:

Constant Biomass:

$(-r) = -dS/dt = k$; (k = constant)

$dt = -dS/k$

$$\int_0^t dt = \int_{So}^{S} -dS/k = (-1/k)\int_{So}^{S} dS$$

$t = (-1/k)(S-So) = So/k - S/k$

$\boxed{t = (-1/k)S + (So/k)}$; (integrated zero-order kinetic expression for constant biomass)

the rate constant, k, can be regressed from experimental S vs. t data using the method of least-squares analysis; regression can be performed with respect to S or t, since the above integrated expression is explicit in both; for the purpose of this study regression is performed with respect to t

One-Parameter: (regress for k only; let So assume the experimental value of S at t = 0)

$t = (-1/k)S + (So/k)$
$= (1/k)(So-S)$

let, $y = t$; (experimental data)
$x = (So-S)$; (experimental data)
$a = (1/k)$ = slope; (regressable parameter)

therefore, $y = ax$

by least-squares analysis (refer to A-17)

$a = \Sigma xy/\Sigma x^2 = (1/k)$

$\boxed{k = (1/a) = \Sigma x^2/\Sigma xy}$

Two-Parameter: (regress for both k and So)

$t = (-1/k)S + (So/k)$

let, $y = t$; (experimental data)
$x = S$; (experimental data)
$a = (-1/k)$ = slope; (regressable parameter)
$b = (So/k)$ = intercept; (regressable parameter)

therefore, $y = ax + b$

by least-squares analysis (refer to A-18)

$a = (n\Sigma xy - \Sigma x \Sigma y)/(n\Sigma x^2 - (\Sigma x)^2)$
$b = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x)/(n\Sigma x^2 - (\Sigma x)^2)$

$$\boxed{k = (-1/a) = (n\Sigma x^2 - (\Sigma x)^2)/(\Sigma x \Sigma y - n\Sigma xy)}$$

$$\boxed{So = (-b/a) = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x)/(\Sigma x \Sigma y - n\Sigma xy)}$$

calculation of S as a function of t is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the integrated zero-order kinetic expression is explicit with respect to S:

$$\boxed{S = So - kt}$$

Zero-Order Kinetics:

Variable Biomass:

$(-r) = -dS/dt = k$; $k = f(\text{biomass concentration})$
$= koB$
$= ko(Bo + Yc(So-S))$

where,

Bo, So, Yc = constants (assumed available)
ko = regressable parameter

$-dS/dt = ko\,(Bo + Yc(So - S))$
$-kodt = dS/(Bo + Yc(So-S)) = dS/(Bo+YcSo-YcS)$

$\int_o^t -kodt = -kot = \int_{So}^{S} dS/(Bo+YcSo-YcS)$

$= (-1/Yc)\int_{So}^{S} (-YcdS)/(Bo+YcSo-YcS)$

$= (-1/Yc)\ln(Bo+YcSo-YcS)\Big|_{So}^{S}$

$= (-1/Yc)(\ln(Bo+YcSo-YcS)-\ln(Bo+YcSo-YcSo))$

$= (-1/Yc)(\ln(Bo+YcSo-YcS)-\ln(Bo))$

$\boxed{t = (1/koYc)(\ln(Bo+YcSo-YcS)-\ln(Bo))}$; (integrated zero-order kinetic expression for variable biomass)

the rate constant, ko, can be regressed from experimental S vs. t data, provided biomass data are available, using the method of least-squares analysis; regression is performed with respect to the explicit variable t

One-Parameter: (regress for ko only; Bo, So, and Yc are assumed given)

$t = (1/koYc)(\ln(Bo+YcSo-YcS)-\ln(Bo))$
$= (1/koYc)(\ln((Bo+YcSo-YcS)/Bo))$

let, $y = t$; (experimental data)
$x = \ln((Bo+YcSo-YcS)/Bo)$; (experimental data)
$a = (1/koYc) = \text{slope}$; (regressable parameter)

therefore, $y = ax$

by least-squares analysis (refer to A-17)

$a = \Sigma xy/\Sigma x^2 = (1/koYc)$

$\boxed{ko = (1/aYc) = \Sigma x^2/(Yc\,\Sigma xy)}$

calculation of S as a function of t is straightforward once ko has been determined since the integrated zero-order kinetic expression for variable biomass is explicit with respect to S:

$$S = (Bo+YcSo-Bo*\exp(koYct))/Yc$$

First-Order Kinetics:

Constant Biomass:

$(-r) = -dS/dt = kS$; (k = constant)

$dt = -dS/(kS)$

$$\int_0^t dt = \int_{S_o}^{S} -dS/(kS) = (-1/k)\int_{S_o}^{S} dS/S$$

$$\boxed{t = (-1/k)\ln(S/So)}$$;(integrated first-order kinetic expression for constant biomass)

the rate constant, k, can be regressed from experimental S vs. t data using the method of least-squares analysis; regression is performed with respect to the explicit variable t

One-Parameter: (regress for k only; let So assume the experimental value of S at t=0)

$t = (-1/k)\ln(S/So)$
$= (1/k)\ln(So/S)$

let, $y = t$; (experimental data)
$x = \ln(So/S)$; (experimental data)
$a = (1/k)$ = slope; (regressable parameter)
therefore, $y = ax$

by least-squares analysis (refer to A-17)

$a = \Sigma xy / \Sigma x^2 = (1/k)$

$$\boxed{k = (1/a) = \Sigma x^2 / \Sigma xy}$$

Two-Parameter: (regress for both k and So)

$$t = (-1/k)\ln(S/So)$$
$$= (1/k)\ln(So/S)$$
$$= (1/k)(\ln So - \ln S)$$
$$= (-1/k)\ln S + ((\ln So)/k)$$

let, $y = t$; (experimental data)
$x = \ln S$; (experimental data)
$a = (-1/k)$ = slope; (regressable parameter)
$b = (\ln So)/k$ = intercept; (regressable parameter)

therefore, $y = ax + b$

by least-squares analysis (refer to A-18)

$$a = (n\Sigma xy - \Sigma x \Sigma y)/(n\Sigma x^2 - (\Sigma x)^2)$$

$$b = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x)/(n\Sigma x^2 - (\Sigma x)^2)$$

$$\boxed{k = (-1/a) = (n\Sigma x^2 - (\Sigma x)^2)/(\Sigma x \Sigma y - n\Sigma xy)}$$

$$\boxed{So = \exp(-b/a) = \exp((\Sigma x^2 \Sigma y - \Sigma xy \Sigma x)/(\Sigma x \Sigma y - n\Sigma xy))}$$

calculation of S as a function of t is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the integrated first-order kinetic expression for constant biomass is explicit with respect to S:

$$\boxed{S = So * \exp(-kt)}$$

First-Order Kinetics:

Variable Biomass:

$$(-r) = -dS/dt = kS;\ k = f(\text{biomass concentration}) = koB = ko(Bo+Yc(So-S))$$

where,

Bo, So, Yc = constants (assumed available)

ko = regressable parameter

$$-dS/dt = ko(Bo+Yc(So-S))S$$

$$-kodt = dS/((Bo+Yc(So-S))S)$$

$$\int_o^t -kodt = -kot = \int_{So}^{S} dS/((Bo+Yc(So-S))S)$$

$$= \int_{So}^{S} dS/((Bo+YcSo-YcS)S)$$

$$= (-1/(Bo+YcSo))\ln((Bo+YcSo-YcS)/S)\Big|_{So}^{S}$$

$$= (-1/(Bo+YcSo))(\ln((Bo+YcSo-YcS)/S) - \ln((Bo+YcSo-YcSo)/So))$$

$$= (-1/(Bo+YcSo))(\ln((Bo+YcSo-YcS)/S) - \ln(Bo/So))$$

$$= (-1/(Bo+YcSo))\ln((Bo+YcSo-YcS)So/(BoS))$$

$$\boxed{t = (-1/(ko(Bo+YcSo)))\ln((BoS)/((Bo+YcSo-YcS)So))}\ ;$$

(integrated first-order kinetic expression for variable biomass)

the rate constant, ko, can be regressed from experimental S vs. t data, provided biomass data are available, using the method of least-squares analysis; regression is performed with respect to the explicit variable t

One-Parameter: (regress for ko only; Bo, So, and Yc are assumed given)

$$t = (-1/(ko(Bo+YcSo)))\ln(BoS/((Bo+YcSo-YcS)So))$$

let, $y = t$; (experimental data)

$x = \ln(BoS/((Bo+YcSo-YcS)So))$; (experimental data)

$a = (-1/(ko(Bo+YcSo))) = \text{slope}$; (regressable parameter)

therefore, $y = ax$

by least-squares analysis (refer to A-17)

$$a = \sum xy / \sum x^2 = (-1/(ko(Bo+YcSo)))$$

$$\boxed{ko = (-1/(a(Bo+YcSo))) = -\sum x^2 / (\sum xy(Bo+YcSo))}$$

calculation of S as a function of t is straightforward once ko has been determined since the integrated first-order kinetic expression for variable biomass is explicit with respect to S:

$$\boxed{S = (Bo+YcSo)/(Yc+(Bo/So)exp((Bo+YcSo)kot))}$$

Monod Kinetics:

Constant Biomass:

$(-r) = -dS/dt = kS/(K+S)$; (k and K are constants)

$dt = -(K+S)dS/Sk$

$$\int_o^t k\,dt = \int_{So}^{S} -(K+S)dS/S = \int_{So}^{S} -(K/S)dS - \int_{So}^{S} dS$$

$$= -K \int_{So}^{S} dS/S - \int_{So}^{S} dS$$

$$= -K \ln S\Big|_{So}^{S} - S\Big|_{So}^{S}$$

$$= -K \ln(S/So) - (S-So)$$

$$\boxed{t = (K/k)\ln(So/S)+(1/k)(So-S)}$$; (integrated Monod kinetic expression for constant biomass)

the rate constants (k and K) can be regressed from experimental S vs. t data using the method of least-squares analysis; regression is performed with respect to the explicit variable t

Two-Parameter: (regress for k and K only; let So assume the expermental value of S at t = 0)

$t = (K/k)\ln(So/S)+(1/k)(So-S)$

let, $y = t$; (experimental data)
$x = \ln(So/S)$; (experimental data)
$z = (So-S)$; (experimental data)
$a = (K/k)$; (regressable parameter)
$b = (1/k)$; (regressable parameter)

therefore, $y = ax + bz$

by least-squares analysis (refer to A-19)

$$a = (\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2) = (K/k)$$

$$b = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2) = (1/k)$$

$$\boxed{k = (1/b) = (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)/(\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)}$$

$$\boxed{K = (a/b) = (\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz)/(\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)}$$

Three-Parameter: (regress for k, K and So)

$$t = (K/k)\ln(So/S) + (1/k)(So-S)$$
$$= (K/k)\ln So - (K/k)\ln S + (So/k) - (S/k)$$
$$= (-K/k)\ln S + (-1/k)S + ((K/k)\ln So + (So/k))$$

let, $y = t$; (experimental data)
$x = \ln S$; (experimental data)
$z = S$; (experimental data)
$a = (-K/k)$; (regressable parameter)
$b = (-1/k)$; (regressable parameter)
$c = ((K/k)\ln So + (So/k))$; (regressable parameter)

therefore, $y = ax + bz + c$

by least-squares analysis (refer to A-20)

$a = (-K/k)$; (see A-22)
$b = (-1/k)$; (see A-22)
$c = (K/k)\ln So + (So/k)$; (see A-22)

$\boxed{k = (-1/b)}$; (see A-22)

$\boxed{K = (a/b)}$; (see A-22)

So, or S for any value of t for either the two- or three-parameter models can be determined by a trial-and-error procedure such as Newton's Rule (refer to A-23) provided the values of k and K are known; straightforward calculation of S is not possible since the integrated Monod expressions are not explicit with respect to S.

Monod Kinetics:

Variable Biomass:

$(-r) = -dS/dt = kS/(K + S)$; K = constant

k = f(biomass concentration)

= koB

= ko(Bo + Yc(So-S))

where,

Bo, So, Yc = constants (assumed available)

ko,K = regressable parameters

$-dS/dt = ko(Bo + Yc(So-S))S/(K + S)$

$-kodt = (K + S)dS/(S(Bo + Yc\ (So-S))$

$\int_o^t -kodt = -kot = \int_{So}^{S} (K + S)dS/(S(Bo + YcSo - YcS))$

$= K\int_{So}^{S} dS/((Bo + YcSo - YcS)S) +$

$\int_{So}^{S} dS/(Bo + YcSo - YcS)$

$= (-K/(Bo + YcSo))\ln((Bo + YcSo - YcS)/S)\Big|_{So}^{S} +$

$(-1/Yc)\ln(Bo + YcSo - YcS)\Big|_{So}^{S}$

$= (-K/(Bo + YcSo))\ln((Bo + YcSo-YcS)/S) -$

$(-K/(Bo + YcSo))\ln((Bo + YcSo - YcSo)/So) +$

$(-1/Yc)\ln(Bo + YcSo - YcS) -$

$(-1/Yc)\ln(Bo + YcSo - YcSo)$

$= (-K/(Bo + YcSo))\ln((Bo + YcSo - YcS)So/(BoS))$

$+ (-1/Yc)\ln((Bo + YcSo - YcS)/Bo)$

$$t = (K/(ko(Bo + YcSo)))\ln((Bo + YcSo-YcS)So/(BoS)) + (1/(koYc))\ln((Bo + YcSo - YcS)/Bo)$$

; (integrated Monod kinetic expression for variable biomass)

the rate constants, ko and K, can be regressed from experimental S vs. t data, provided biomass data are available, using the method of least-squares analysis; regression is performed with respect to the explicit variable t

Two-Parameter: (regress for ko and K; Bo, Yc and So are assumed given)

$$t = (K/(ko(Bo + YcSo)))\ln((Bo + YcSo - YcS)So/(BoS)) + (1/(koYc))\ln((Bo + YcSo - YcS)/Bo)$$

let, $y = t$; (experimental data)

$x = \ln((Bo + YcSo - YcS)So/(BoS))$; (experimental data)

$z = \ln((Bo + YcSo - YcS)/Bo)$; (experimental data)

$a = (K/(ko(Bo + YcSo)))$; (regressable parameter)

$b = (1/(koYc))$; (regressable parameter)

therefore, $y = ax + bz$

by least-square analysis (refer to A-19)

$$a = (\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2) = (K/(ko(Bo + YcSo)))$$

$$b = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2) = (1/(koYc))$$

$$\boxed{ko = (1/bYc) = (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)/(Yc(\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz))}$$

$$\boxed{K = (a(Bo + YcSo))/(bYc) = ((\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz)(Bo + YcSo))/((\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)Yc)}$$

calculation of S as a function of t can be determined by a trial-and-error procedure (once the regressable parameters have been determined) such as Newton's Rule (refer to A-23); straight-forward calculation of S is not possible since the integrated Monod expression for variable biomass is not explicit with respect to S

Method of Least-Squares Analysis: Derivations

Case 1: $Y = ax$

given a set of data (i.e., y as a function of x) it can be fit to an algebraic expression $Y = ax$

let, E = error

$$= y - Y = y - (ax) = y - ax$$

"a" should be chosen such that the sum of the square of the error, ΣE^2 (or f(a)), is minimized

$$f(a) = \Sigma E^2 = \Sigma (y - ax)^2$$

$$df(a)/da = d(\Sigma (y-ax)^2)/da$$

$$= 2\Sigma (y-ax)(-x)$$

$$= 0$$

therefore, $\Sigma xy - a\Sigma x^2 = 0$; $\boxed{a = \Sigma xy/\Sigma x^2}$

Case 2: $Y = ax + b$

given a set of data (i.e., y as a function of x), it can be fit to an algebraic expression $Y = ax + b$

let, E = error
$= y-Y = y-(ax + b) = y-ax-b$

"a" and "b" should be chosen such that the sum of the square of the error, ΣE^2 (or f(a, b)), is minimized

$$f(a,b) = \Sigma E^2 = \Sigma(y-ax-b)^2$$

$$\partial f(a,b)/\partial a = \partial/\partial a\,(\Sigma(y-ax-b)^2) = 2\Sigma(y-ax-b)(-x) = 0$$

$$\partial f(a,b)/\partial b = \partial/\partial b(\Sigma(y-ax-b)^2) = 2\Sigma(y-ax-b)(-1) = 0$$

therefore, $\Sigma xy - a\Sigma x^2 - b\Sigma x = 0$
$\Sigma y - a\Sigma x - nb = 0;$
(n = # of data points)

simultaneous solution of the above two equations for the two unknowns (i.e., a and b) algebraically yields:

$$\boxed{a = (n\Sigma xy - \Sigma x\,\Sigma y)/(n\Sigma x^2 - (\Sigma x)^2)}$$

$$\boxed{b = (\Sigma x^2\Sigma y - \Sigma xy\,\Sigma x)/(n\Sigma x^2 - (\Sigma x)^2)}$$

Case 3: $Y = ax + bz$

given a set of data (i.e., y as a function of x and z), it can be fit to an algebraic expression $Y = ax + bz$

let, E = error

$$= y - Y = y-(ax + bz) = y - ax - bz$$

"a" and "b" should be chosen such that the sum of the square of the error, ΣE^2 (or f(a,b)), is minimized

$$f(a,b) = \Sigma E^2 = \Sigma (y - ax - bz)^2$$

$$\partial f(a,b)/\partial a = \partial/\partial a \, (\Sigma(y - ax - bz)^2)$$
$$= 2\Sigma(y - ax - bz)(-x)$$
$$= 0$$

$$\partial f(a,b)/\partial b = \partial/\partial b(\Sigma(y - ax - bz)^2)$$
$$= 2\Sigma(y - ax - bz)(-z)$$
$$= 0$$

therefore, $\Sigma xy - a\Sigma x^2 - b\Sigma xz = 0$
$\Sigma yz - a\Sigma xz - b\Sigma z^2 = 0$

simultaneous solution of the above two equations for the two unknowns (i.e., a and b) algebraically yields:

$$\boxed{a = (\Sigma xy \Sigma z^2 - \Sigma yz \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)}$$

$$\boxed{b = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)}$$

Case 4: $Y = ax + bz + c$

given a set of data (i.e., y as a function of x and z), it can be fit to an algebraic expression $Y = ax + bz + c$

let, E = error

$$= y - Y = y - (ax + bz + c)$$

$$= y - ax - bz - c$$

"a", "b", and "c" should be chosen such that the sum of the square of the error, ΣE^2 (or $f(a,b,c)$) is minimized

$$f(a,b,c) = \Sigma E^2 = \Sigma(y - ax - bz - c)^2$$
$$\partial f(a,b,c)/\partial a = \partial/\partial a\ (\Sigma(y - ax - bz - c)^2)$$
$$= 2\Sigma(y - ax - bz - c)\ (-x)$$
$$= 0$$
$$\partial f(a,b,c)/\partial b = \partial/\partial b\ (\Sigma(y - ax - bz - c)^2)$$
$$= 2\Sigma(y - ax - bz - c)\ (-z)$$
$$= 0$$
$$\partial f(a,b,c)/\partial c = \partial/\partial c\ (\Sigma(y - ax - bz - c)^2)$$
$$= 2\Sigma(y - ax - bz - c)\ (-1)$$
$$= 0$$

therefore,
$$\Sigma xy - a\Sigma x^2 - b\Sigma x\, z - c\Sigma x = 0$$
$$\Sigma yz - a\Sigma xz - b\Sigma z^2 - c\Sigma z = 0$$
$$\Sigma y - a\Sigma x - b\Sigma z - nc = 0$$
(n = # of data points)

simultaneous solution of the above three equations for the three unknowns (i.e., a, b, and c) can be accomplished using matrix algebra

rewrite the above equations,

$$(\Sigma x^2)\ a + (\Sigma xz)\ b + (\Sigma x)c = \Sigma xy$$
$$(\Sigma xz)\ a + (\Sigma z^2)\ b + (\Sigma z)c = \Sigma yz$$
$$(\Sigma x)\ a + (\Sigma z)\ b + (n)\ c = \Sigma y$$

redefine the equations,

$$(A1)\ a + (B1)\ b + (C1)\ c = D1$$
$$(A2)\ a + (B2)\ b + (C2)\ c = D2$$
$$(A3)\ a + (B3)\ b + (C3)\ c = D3$$

where,

$A1 = \Sigma x^2$; $B1 = \Sigma xz$; $C1 = \Sigma x$; $D1 = \Sigma xy$
$A2 = \Sigma xz$; $B2 = \Sigma z^2$; $C2 = \Sigma z$; $D2 = \Sigma yz$
$A3 = \Sigma x$; $B3 = \Sigma z$; $C3 = n$; $D3 = \Sigma y$

therefore the matrix can be written:

$$\left[\begin{array}{ccc|c} A1 & B1 & C1 & D1 \\ A2 & B2 & C2 & D2 \\ A3 & B3 & C3 & D3 \end{array}\right]$$

divide row 1 by A1, row 2 by A2, and row 3 by A3,

$$\left[\begin{array}{ccc|c} 1 & B1/A1 & C1/A1 & D1/A1 \\ 1 & B2/A2 & C2/A2 & D2/A2 \\ 1 & B3/A3 & C3/A3 & D3/A3 \end{array}\right]$$

substract row 1 from both rows 2 and 3,

$$\left[\begin{array}{ccc|c} 1 & B1/A1 & C1/A1 & D1/A1 \\ 0 & B2/A2-B1/A1 & C2/A2-C1/A1 & D2/A2-D1/A1 \\ 0 & B3/A3-B1/A1 & C3/A3-C1/A1 & D3/A3-D1/A1 \end{array}\right]$$

rewrite the above matrix,

$$\left[\begin{array}{ccc|c} 1 & E1 & F1 & G1 \\ 0 & E2 & F2 & G2 \\ 0 & E3 & F3 & G3 \end{array}\right]$$

where, $E1 = B1/A1$; $F1 = C1/A1$; $G1 = D1/A1$
$E2 = B2/A2-E1$; $F2 = C2/A2 - F1$; $G2 = D2/A2 - G1$
$E3 = B3/A3-E1$; $F3 = C3/A3 - F1$; $G3 = D3/A3 - G1$

divide row 2 by E2 and row 3 by E3,

$$\left[\begin{array}{ccc|c} 1 & E1 & F1 & G1 \\ 0 & 1 & F2/E2 & G2/E2 \\ 0 & 1 & F3/E3 & G3/E3 \end{array}\right]$$

subtract row 2 multiplied by E1 from row 1; subtract row 2, as is, from row 3,

$$\left[\begin{array}{ccc|c} 1 & 0 & F1 - F2*(E1/E2) & G1-G2*(E1/E2) \\ 0 & 1 & F2/E2 & G2/E2 \\ 0 & 0 & F3/E3 - F2/E2 & G3/E3 - G2/E2 \end{array}\right]$$

rewrite the above matrix,

$$\left[\begin{array}{ccc|c} 1 & 0 & H1 & I1 \\ 0 & 1 & H2 & I2 \\ 0 & 0 & H3 & I3 \end{array}\right]$$

where, $H1 = F1 - E1 * H2$; $I1 = G1 - E1 * I2$
$H2 = F2/E2$; $I2 = G2/E2$
$H3 = F3/E3 - H2$; $I3 = G3/E3 - I2$

divide row 3 by H3,

$$\left[\begin{array}{ccc|c} 1 & 0 & H1 & I1 \\ 0 & 1 & H2 & I2 \\ 0 & 0 & 1 & I3/H3 \end{array}\right]$$

subtract row 3, multiplied by H1, from row 1;
subtract row 3, multiplied by H2, from row 2,

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & I1 - H1 * I3/H3 \\ 0 & 1 & 0 & I2 - H2 * I3/H3 \\ 0 & 0 & 1 & I3/H3 \end{array}\right]$$

therefore,

$$\boxed{\begin{array}{l} a = I1 - I3 * H1/H3 \\ b = I2 - I3 * H2/H3 \\ c = I3/H3 \end{array}}$$

where, $H1 = F1 - E1 * H2$; $I1 = G1 - E1 * I2$
$H2 = F2/E2$; $I2 = G2/E2$
$H3 = F3/E3 - H2$; $I3 = G3/E3 - I2$

where, $E1 = B1/A1$; $F1 = C1/A1$; $G1 = D1/A1$
$E2 = B2/A2 - E1$; $F2 = C2/A2 - F1$; $G2 = D2/A2 - G1$
$E3 = B3/A3 - E1$; $F3 = C3/A3 - F1$; $G3 = D3/A3 - G1$

where, $A1 = \Sigma x^2$; $B1 = \Sigma xz$; $C1 = \Sigma x$; $D1 = \Sigma xy$
$A2 = \Sigma xz$; $B2 = \Sigma z^2$; $C2 = \Sigma z$; $D2 = \Sigma yz$
$A3 = \Sigma x$; $B3 = \Sigma z$; $C3 = n$; $D3 = \Sigma y$

Newton's Rule:

This technique is used for finding a root of a single-variable non-linear equation, such as any of the following three forms of the integrated Monod kinetics:

(1a): $t = (K/k)\ln(So/S)+(1/k)(So-S)$; constant biomass (2-parameter)
$= a \ln(So/S)+ b (So-S)$; (refer to A-13)

(2a): $t = (-K/k)\ln S+(-1/k)S+((K/k)\ln So+So/k)$; constant biomass (3-par.)
$= a \ln S+ b S + c$; (refer to A-14)

(3a): $t = (K/(ko(Bo+YcSo)))\ln((Bo+YcSo-YcS)So/(BoS))+(1/(koYc))$
$\ln((Bo+YcSo-YcS)/Bo)$; variable biomass (2-parameter)
$= a \ln((Bo+YcSo-YcS)So/(BoS))+ b \ln((Bo + YcSo-YcS)/Bo)$;
(refer to A-16)

Rewrite each expression as a function of S equal to zero:

(1b): $f(S) = a \ln(S/So) + b(S-So) + t = 0$

(2b): $f(S) = a \ln S + b S + c - t = 0$

(3b): $f(S) = a\ln((Bo+YcSo-YcS)So/(BoS))+b\ln((Bo + YcSo - YcS)/Bo)-t = 0$

For the above three expressions, a, b, c, So, Bo and Yc are assumed given while S is to be determined for various values of t.

The first derivatives of each of the above three expressions are:

(1c): $f'(S) = a/S + b = 0$

(2c): $f'(S) = a/S + b = 0$

(3c): $f'(S) =-(a+b)Yc/(Bo+YcSo-YcS) - a/S = 0$

The solution of S for a given t may be multiple (i.e., more than one root). To get the desired root requires a good initial guess of S--So is usually a good value to use. Once the initial value of S is chosen, an iterative procedure is used to calculate subsequent values of S until the difference between the new and old value is negligible. For this study, the convergence value (i.e., new value minus old value) was arbitrarily chosen to be 0.0001.

Let, $S_i = S_o$

$S_{i+1} = S_i - f(S_i)/f'(S_i)$

if $|S_{i+1} - S_i| < 0.0001$, $S = S_{i+1}$!

if not, let $S_i = S_{i+1}$ and repeat the above calculations until the convergence value is attained

For the purpose of this study, a simple program was written in BASIC for the SHARP PC-1500 pocket computer to calculate S for various values of t This program is listed below:

```
 5:  S = 0  : SN = 0 : T = 0 : FS = 0 : FPS = 0
10:  A2 = 0 : B2 = 0 : S0 = 0
15:  A3 = 0 : B3 = 0 : C3 = 0
20:  AV = 0 : BV = 0 : B0 = 0 : YC = 0
25:  INPUT "a(2-parameter; constant) =", A2
30:  INPUT "b(2-parameter; constant) =", B2
35:  INPUT "So = ", S0
40:  INPUT "a(3-parameter; constant) =", A3
45:  INPUT "b(3-parameter; constant) =", B3
50:  INPUT "c(3-parameter; constant) =", C3
55:  INPUT "a(2-parameter; variable) =", AV
60:  INPUT "b(2-parameter; variable) =", BV
65:  INPUT "Bo =", B0
70:  INPUT "Yc =", YC
75:  S = S0
80:  FS = A2*LN(S/S0)+B2*(S-S0)+T
85:  FPS = A2/S + B2
90:  SN = S - FS/FPS
95:  IF ABS (SN-S)<1E-4 THEN GOTO 110
100: S = SN
105: GOTO 80
110: PRINT "MONOD 2-PARAMETER (CONST)"
115: PRINT "t = "; T; ";S = "; SN
120: IF T = 6 THEN GOTO 135
125: T = T + 0.25
130: GOTO 100
135: T = 0
140: S = S0
145: FS = A3*LNS + B3*S+C3-T
150: FPS = A3/S + B3
155: SN = S - FS/FPS
160: IF ABS(SN - S)<1E-4 THEN GOTO 175
165: S = SN
170: GOTO 145
175: PRINT "MONOD 3-PARAMETER (CONST)"
180: PRINT "t = "; T; "; S = "; SN
185: IF T = 6 THEN GOTO 200
190: T = T + 0.25
195: GOTO 165
```

```
200: T = 0
205: S = SO
210: FS = AV*LN((BO+YC*SO-YC*S)*SO/(BO*S))
          + BV*LN((BO+YC*SO-YC*S)/BO)-T
215: FPS =-(AV+BV)*YC/(BO+YC*SO-YC*S)-AV/S
220: SN = S - FS/FPS
225: IF ABS(SN-S)<1E-4 THEN GOTO 240
230: S = SN
235: GOTO 210
240: PRINT "MONOD 2-PARAMETER (VAR)"
245: PRINT "t = "; T; "; S = "; SN
250: IF T = 6 THEN GOTO 265
255: T = T + 0.25
260: GOTO 230
265: END
```

The above program requires that the results from the regression analyses for each form of Monod equation be inputted upon request of the pocket computer (as specified by the program):

```
2-parameter model (constant biomass)→a,b,So
3-parameter model (constant biomass)→a,b,c
2-parameter model (variable biomass)→a,b,Bo,Yc
```

The program will calculate values of S for corresponding values of t from 0 to 6 hours in 1/4-hour increments for the 2-parameter constant biomass model first, then the 3-parameter model, and then finally the 2-parameter variable-biomass model. The units for S in this study are parts per million (ppm).

To calculate S for a single value of t, rather than the above range, modify the above program as indicated below. Insert the following program statement:

```
76:  INPUT "t=", T
```

Delete the following program statements: 120, 125, 130, 135, 140, 185, 190, 195, 200, 205, 250, 255, 260.

To calculate S for multiple values of t without reinputting the regressed results every time, insert the following program statement:

```
264:  GOTO 76
```

The last modification will require the program to be manually terminated once all the desired results are attained, since an infinite loop exists.

Appendix B

Mathematical Derivation of Kinetic Expressions for the Regression of Biodegradation Rate Constants from Continuous Stirred-Tank Reactor Data (i.e., CSTR)

Table of Contents

Nomenclature

a,b,c = regressable parameters

A,B,C = miscellaneous variables (as defined on B-10 and B-14)

Be = biomass concentration = Bi + Yc(Si-Se)

Bi = initial biomass concentration

k = biodegradation rate constant = koBe

K = constant for Monod kinetic expression

ko = biodegradation rate constant (independent of biomass concentration)

Q = volumetric flow rate

Qe = effluent volumetric flow rate

Qi = inlet volumetric flow rate

(-r) = biodegradation rate (ppm/hr.)

Se = effluent substrate concentration (ppm)

Si = feed substrate concentration (ppm)

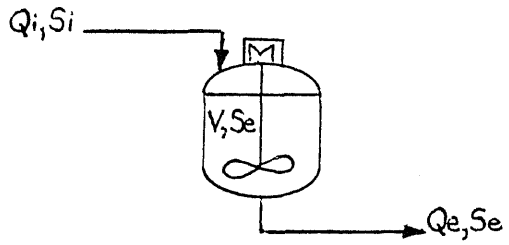
V = reactor volume

x,y,z = variables used in regression analyses

Yc = yield coefficient = (Be-Bi)/(Si-Se)

τ = (V/Q) = reactor time constant

Ideal Continuous Stirred-Tank Reactor: (Performance Eqn.)



assume:

i. steady state
ii. uniform composition throughout reactor
iii. constant reactor volume

mass balance: input = output + disappearance + accumulation (0)

input-output = disappearance by reaction

$Q_iS_i - Q_eS_e = (-r)V$

$(S_i-S_e)/(-r) = V/Q$; $(Q_i = Q_e = Q)$

therefore, $\boxed{\tau = (V/Q) = (S_i-S_e)/(-r)}$; performance equation

Zero-Order Kinetics:

Constant Biomass:

$(-r) = (Si-Se)/\tau = k$; (k = constant)

$(Si-Se) = k\tau$

$\boxed{\tau = (-1/k)Se + (Si/k)}$; (zero-order kinetic expression for constant biomass)

the rate constant, k, can be regressed from experimental Se vs. τ (i.e., V/Q) data using the method of least-squares analysis; regression can be performed with respect to Se or τ since the above expression is explicit in both; for the purpose of this study, regression is performed with respect to τ

One-Parameter: (regress for k only; let Si assume the experimental value of the feed substrate concentration)

$\tau = (Si-Se)/k$
$\tau = (1/k)(Si-Se)$

let, $y = \tau = (V/Q)$; (experimental data)
$x = (Si-Se)$; (experimental data)
$a = (1/k) = \text{slope}$; (regressable parameter)

therefore, $y = ax$

by least-squares analysis (refer to A-17)

$a = \Sigma xy / \Sigma x^2 = (1/k)$

$\boxed{k = (1/a) = \Sigma x^2 / \Sigma xy}$

Two-Parameter: (regress for k and Si; this is applicable only for data where the actual feed substrate concentration is held constant--otherwise, the one-parameter model must be used)

$\tau = (-1/k)Se + (Si/k)$

let, $y = \tau = (V/Q)$; (experimental data)
$x = Se$; (experimental data)
$a = (-1/k)$ = slope ; (regressable parameter)
$b = (Si/k)$ = intercept ; (regressable parameter)

therefore, $y = ax + b$

by least-squares analysis (refer to A-18)

$a = (n\Sigma xy - \Sigma x \Sigma y)/(n \Sigma x^2 - (\Sigma x)^2)$
$b = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x)/(n \Sigma x^2 - (\Sigma x)^2)$

$$\boxed{k = (-1/a) = (n \Sigma x^2 - (\Sigma x)^2)/(\Sigma x \Sigma y - n \Sigma xy)}$$

$$\boxed{Si = (-b/a) = (\Sigma x^2 \Sigma y - \Sigma xy \Sigma x)/(\Sigma x \Sigma y - n \Sigma xy)}$$

calculation of Se as a function of τ is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the zero-order kinetic expression is explicit with respect to Se:

$$\boxed{Se = Si - k\tau}$$

Zero-Order Kinetics:

Variable Biomass:

$(-r) = (Si - Se)/\tau = k$; $k = f(\text{biomass concentration})$
$= koBe$
$= ko(Bi + Yc(Si - Se))$

where,

Bi,Si,Yc = constants (assumed available)
ko = regressable parameter

$(-r) = (Si-Se)/\tau = ko(Bi + Yc(Si-Se))$

$$\boxed{\tau = (Si - Se)/(ko(Bi + Yc(Si-Se)))}$$; (zero-order kinetic expression for variable biomass)

the rate constant, ko, can be regressed from experimental Se vs.τ(i.e., V/Q) data using the method of least-squares analysis, provided biomass data are available; regression is performed with respect to the explicit variable τ

One-Parameter: (regress for ko only; Bi,Si, and Yc are assumed given)

$\tau = (1/ko)((Si-Se)/(Bi + Yc(Si-Se)))$

where,

y = (V/Q) ; (experimental data)
x = (Si - Se)/(Bi + Yc(Si-Se)) ; (experimental data)
a = (1/ko) = slope ; (regressable parameter)

therefore, y = ax

by least-squares analysis (refer to A-17)

$a = \Sigma xy/\Sigma x^2 = (1/ko)$

$$\boxed{ko = (1/a) = \Sigma x^2/\Sigma xy}$$

calculation of Se as a function of τ is straightforward once ko has been determined since the zero-order kinetic expression for variable biomass is explicit with respect to Se:

$$\boxed{Se = Si - (ko\,\tau\,Bi)/(1 - ko\,\tau\,Yc)}$$

First-Order Kinetics:

Constant Biomass:

$(-r) = (Si-Se)/\tau = kSe$; (k = constant)

$(Si-Se)/Se = k\tau$

$\boxed{\tau = (1/k)((Si-Se)/Se)}$; (first-order kinetic expression for constant biomass)

the rate constant, k, can be regressed from experimental Se vs. τ(i.e., V/Q) data using the method of least-squares analysis; regression is performed with respect to the explicit variable τ

One-Parameter: (regress for k only; let Si assume the experimental value of the feed substrate concentration)

$\tau = (1/k)((Si-Se)/Se)$

let,

$y = \tau = (V/Q)$; (experimental data)
$x = ((Si-Se)/Se)$; (experimental data)
$a = (1/k) = slope$; (regressable parameter)

therefore, $y = ax$

by least-squares analysis (refer to A-17)

$a = \Sigma xy / \Sigma x^2 = (1/k)$

$\boxed{k = (1/a) = \Sigma x^2 / \Sigma xy}$

Two-Parameter: (regress for k and Si; this is applicable only for data where the actual feed substrate concentration is held constant--otherwise, the one-parameter model must be used)

$\tau = (1/k)((Si-Se)/Se)$
$= (1/k)((Si/Se)-1)$
$= (Si/k)(1/Se) + (-1/k)$

let,

$y = \tau = (V/Q)$; (experimental data)
$x = (1/Se)$; (experimental data)
$a = (Si/k)$ = slope ; (regressable parameter)
$b = (-1/k)$ = intercept ; (regressable parameter)

therefore, $y = ax + b$

by least-squares analysis (refer to A-18)

$$a = (Si/k) = (n\Sigma xy - \Sigma x\,\Sigma y)/(n\Sigma x^2 - (\Sigma x)^2)$$
$$b = (-1/k) = (\Sigma x^2\,\Sigma y - \Sigma xy\,\Sigma x)/(n\Sigma x^2 - (\Sigma x)^2)$$

$$\boxed{k = (-1/b) = (n\Sigma x^2 - (\Sigma x)^2)/(\Sigma xy\,\Sigma x - \Sigma x^2\,\Sigma y)}$$

$$\boxed{Si = (-a/b) = (n\Sigma xy - \Sigma x\,\Sigma y)/(\Sigma xy\,\Sigma x - \Sigma x^2\,\Sigma y)}$$

calculation of Se as a function of τ is straightforward (once the regressable parameters have been determined) for either the one- or two-parameter models since the first-order kinetic expression is explicit with respect to Se:

$$\boxed{Se = Si/(1 + k\tau)}$$

First-Order Kinetics:

Variable Biomass:

$(-r) = (Si-Se)/\tau = kSe$; $k = f(\text{biomass concentration})$
$= koBe$
$= ko(Bi + Yc(Si-Se))$

where,
Bi, Si, Yc = constants (assumed available)
ko = regressable parameter

$(-r) = (Si-Se)/\tau = ko(Bi + Yc\ (Si-Se))Se$

$\boxed{\tau = (1/ko)((Si-Se)/((Bi + Yc\ (Si-Se))Se))}$; (first-order kinetic expression for variable biomass)

the rate constant, ko, can be regressed from experimental Se vs. τ (i.e., V/Q) data using the method of least-squares analysis, provided biomass data are available;regression is performed with respect to the explicit variable τ

One-Parameter: (regress for ko only; Bi, Si and Yc are assumed given)

$\tau = (1/ko)((Si-Se)/((Bi + Yc(Si-Se))Se))$

let,
$y = \tau = (V/Q)$; (experimental data)
$x = (Si-Se)/((Bi + Yc(Si-Se))Se)$; (experimental data)
$a = (1/ko) = \text{slope}$; (regressable parameter)

therefore, $y = ax$

by least-squares analysis (refer to A-17)

$a = (1/ko) = \sum xy / \sum x^2$

$\boxed{ko = (1/a) = \sum x^2 / \sum xy}$

the first-order kinetic expression for variable biomass is a linear 2nd-order polynomial with respect to Se; as such, the calculation of Se as a function of τ can be accomplished (providing ko has been determined) by using the quadratic formula:

$\boxed{Se^2\ (Ycko\tau) + Se\ (-1-YcSiko\tau - Biko\tau) + (Si) = 0}$

where, $A = (Ycko\tau)$
$B = (-1-YcSiko\tau - Biko\tau)$
$C = (Si)$

therefore, $\boxed{Se = (-B \pm (B^2 - 4AC)^{0.5})/(2A)}$

Monod Kinetics:

Constant Biomass:

$(-r) = (Si-Se)/\tau = kSe/(K + Se)$; (k and K are constants)

$\tau = (Si-Se)(K + Se)/(Sek)$

$$\boxed{\tau = ((Si-Se)(K + Se))/(kSe)}$$; (Monod kinetic expression for constant biomass)

the rate constants (k and K) can be regressed from experimental Se vs. τ (i.e., V/Q) data using the method of least-squares analysis; regression is performed with respect to the explicit variable τ

Two-Parameter: (regress for k and K only; let Si assume the experimental value of the feed substrate concentration)

$$\begin{aligned}\tau &= ((Si-Se)(K + Se))/(kSe)\\ &= (Si-Se)K/(kSe) + (Si-Se)Se/(kSe)\\ &= (K/k)((Si-Se)/Se) + (1/k)(Si-Se)\end{aligned}$$

let,

$y = \tau = (V/Q)$; (experimental data)
$x = ((Si-Se)/Se)$; (experimental data)
$z = (Si-Se)$; (experimental data)
$a = (K/k)$; (regressable parameter)
$b = (1/k)$; (regressable parameter)

therefore, $y = ax + bz$

by least-squares analysis (refer to A-19)

$$a = (K/k) = (\Sigma xy \Sigma z^2 - \Sigma yz \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2$$
$$b = (1/k) = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2$$

$$\boxed{k = (1/b) = (\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)/(\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz}$$

$$\boxed{K = (a/b) = (\Sigma xy \Sigma z^2 - \Sigma yz \Sigma xz)/(\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)}$$

Three-Parameter: (regress for k, K and Si; this is applicable only for data where the actual feed substrate concentration is held constant--otherwise the two-parameter model must be used)

$$\tau = ((Si-Se)(K + Se))/(kSe)$$
$$= (SiK + (Si-K)Se-Se^2)/(kSe)$$
$$= (SiK/k)(1/Se) + (Si-K)/k - (1/k)Se$$
$$= (SiK/k)(1/Se) + (-1/k)\ Se + ((Si-K)/k)$$

let,
$y = \tau = (V/Q)$; (experimental data)
$x = (1/Se)$; (experimental data)
$z = Se$; (experimental data)
$a = (SiK/k)$; (regressable parameter)
$b = (-1/k)$; (regressable parameter)
$c = ((Si-K)/k)$; (regressable parameter)

therefore, $y = ax + bz + c$

by least-squares analysis (refer to A-20)

$a = (SiK/k)$; (see A-22)
$b = (-1/k)$; (see A-22)
$c = ((Si-K)/k)$; (see A-22)

$$\boxed{k = (-1/b)} \text{ ; (see A-22)}$$

$$\boxed{K = (c \pm (c^2 - 4\ ba)^{0.5})/(2b)} \text{ ; (see A-22)}$$

$$\boxed{Si = (-c \pm (c^2 - 4ba)^{0.5})/(2b)} \text{ ; (see A-22)}$$

the Monod kinetic expression for constant biomass is a linear 2nd-order polynomial with respect to Se; as such, the calculation of Se as a function of τ can be accomplished (once the regressable parameters have been determined) by using the quadratic formula:

$$\boxed{Se = (-(k\tau + K-Si) \pm ((k\tau + K - Si)^2 + 4SiK)^{0.5})/2}$$

Monod Kinetics:

Variable Biomass:

$(-r) = (Si-Se)/\tau = kSe/(K + Se)$; k = f(biomass concentration)
= koBe
= ko(Bi + Yc(Si-Se))

where,
Bi,Si,Yc = constants (assumed available)
ko = regressable parameter

$(-r) = (Si-Se)/\tau = ko(Bi + Yc(Si-Se))Se/(K + Se)$

$\boxed{\tau = (1/ko)(Si-Se)(K + Se)/((Bi + Yc(Si-Se))Se)}$; (Monod kinetic expression for variable biomass

the rate constants (ko and K) can be regressed from experimental Se vs. τ (i.e., V/Q) data using the method of least-squares analysis, provided biomass data are available; regression is performed with respect to the explicit variable τ

Two-Parameter: (regress for ko and K only; Bi,Si and Yc are assumed given)

$\tau = (K/ko)((Si-Se)/((Bi+Yc(Si-Se))Se)) + (1/ko)((Si-Se)/(Bi + Yc(Si - Se)))$

let,
$y = \tau = (V/Q)$; (experimental data)
$x = ((Si-Se)/((Bi + Yc(Si-Se))Se))$; (experimental data)
$z = ((Si-Se)/(Bi + Yc(Si-Se)))$; (experimental data)
$a = (K/ko)$; (regressable parameter)
$b = (1/ko)$; (regressable parameter)

therefore, $y = ax + bz$

by least-squares analysis (refer to A-19)

$$a = (K/ko) = (\Sigma xy\,\Sigma z^2 - \Sigma yz\,\Sigma xz)/(\Sigma x^2\,\Sigma z^2 - (\Sigma xz)^2)$$

$$b = (1/ko) = (\Sigma yz\,\Sigma x^2 - \Sigma xy\,\Sigma xz)/(\Sigma x^2\,\Sigma z^2 - (\Sigma xz)^2)$$

$$\boxed{ko = (1/b) = (\Sigma x^2\,\Sigma z^2 - (\Sigma xz)^2)/(\Sigma yz\,\Sigma x^2 - \Sigma xy\,\Sigma xz)}$$

$$\boxed{K = (a/b) = (\Sigma xy\,\Sigma z^2 - \Sigma yz\,\Sigma xz)/(\Sigma yz\,\Sigma x^2 - \Sigma xy\,\Sigma xz)}$$

the Monod kinetic expression for variable biomass is a linear 2nd-order polynomial with respect to Se; as such, the calculation of Se as a function of τ can be accomplished (once the regressable parameters have been determined) by using the quadratic formula:

$$\boxed{Se^2\,(1 - ko\,Yc\,\tau) + Se\,(Biko\,\tau + Yc\,Siko\,\tau + K - Si) + (-Si\,K) = 0}$$

let, $A = (1 - ko\,Yc\,\tau)$
$B = (Biko\,\tau + Yc\,Siko\,\tau + K - Si)$
$C = (-Si\,K)$

therefore, $\boxed{Se = (-B \pm (B^2 - 4AC)^{0.5})/(2A)}$

Appendix C

Sample Hand Calculations and LOTUS 123 Spreadsheets for the Regression of Batch Reactor Data

Table of Contents

Sample Hand Calculations

Batch Reactor Data Analysis:

Raw Data* - Bo = 19.3 ppm**
Yc = 0.136

t(hr)	S(ppm)
0	160
1	150
9	140
12	110
13	80
15	90
19	20
28	10

* Literature reference: Klecka, G.M., et al. (refer to page D-4).
**Refer to A-3 for clarification of nomenclature.

Zero-Order Kinetics (Constant Biomass)

One-Parameter Model: $t = (1/k)(So-S)$; (refer to A-5)
$y = a \quad x$

y=t	x=So-S	xy	x^2	yc=tc=ax	(t-tc)^2	Sc = So-kt
0	0	0	0	0	0	160
1	10	10	100	1.7	0.49	154
9	20	180	400	3.5	30.25	108
12	50	600	2500	8.6	11.56	91
13	80	1040	6400	13.8	0.64	85
15	70	1050	4900	12.1	8.41	73
19	140	2660	19600	24.2	27.04	50
28	150	4200	22500	25.9	4.41	-2
		Σ=9740	Σ=56400		Σ=82.80	

$a = \Sigma xy/\Sigma x^2 = 9740/56400 = 0.1727$ hr/ppm

$\boxed{k = (1/a) = 5.79 \text{ ppm/hr}}$

Zero-Order Kinetics (Constant Biomass)

Two-Parameter Model: $t = (-1/k)S + (So/k)$; (refer to A-6)
$y = a\ x + b$

y=t	x=S	xy	x^2	yc=tc=ax+b	(t-tc)^2	Sc = So-kt
0	160	0	25600	2.2	4.84	175
1	150	150	22500	3.8	7.84	168
9	140	1260	19600	5.3	13.69	116
12	110	1320	12100	9.8	4.84	96
13	80	1040	6400	14.4	1.96	89
15	90	1350	8100	12.9	4.41	76
19	20	380	400	23.5	20.25	50
28	10	280	100	25.0	9.00	-9
Σ=97	Σ=760	Σ=5780	Σ=94800		Σ=66.83	

$a = (n\Sigma xy-\Sigma x\Sigma y)/(n\Sigma x^2-(\Sigma x)^2)$
$= (8(5780)-(760)(97))/(8(94800)-(760)^2)$
$= -0.1520$ hr./ppm

$b = (\Sigma x^2\Sigma y-\Sigma xy\Sigma x)/(n\Sigma x^2-(\Sigma x)^2)$
$= ((94800)(97)-(5780)(760))/(8(94800)-(760)^2)$
$= 26.564$ hr.

$\boxed{k = (-1/a) = 6.579 \text{ ppm/hr.}}$

$\boxed{So = (-b/a) = 174.8 \text{ ppm}}$

First-Order Kinetics (Constant Biomass)

One-Parameter Model: $t = (1/k)\ln(So/S)$; (refer to A-9)
$y = a \quad x$

y=t	x=ln(So/S)	xy	x^2	yc=tc=ax	(t-tc)^2	Sc = f(t)*
0	0	0	0	0	0	160
1	0.0645	0.0645	0.0042	0.7	0.09	146
9	0.1335	1.2015	0.0178	1.4	57.76	70
12	0.3747	4.4964	0.1404	4.1	62.41	53
13	0.6931	9.0103	0.4804	7.5	30.25	48
15	0.5754	8.6310	0.3311	6.2	77.44	40
19	2.0794	39.5094	4.3239	22.5	12.25	28
28	2.7726	77.6325	7.6873	30.0	4.00	12
		Σ=140.55	Σ=12.985		Σ=244.20	

$a = \Sigma xy/\Sigma x^2 = 140.55/12.985 = 10.82$ hr.

$\boxed{k = (1/a) = 0.0924/hr.}$

* $Sc = So*\exp(-kt)$

First-Order Kinetics (Constant Biomass)

Two-Parameter Model: $t = (-1/k)\ln S+((\ln So)/k)$; (refer to A-10)

$y = a\ x + b$

y=t	x=lnS	xy	x^2	yc=tc=ax+b	(t-tc)^2	Sc = f(t)*
0	5.0752	0	25.758	5.4	29.16	313
1	5.0106	5.011	25.106	5.9	24.01	276
9	4.9416	44.474	24.419	6.5	6.25	102
12	4.7005	56.406	22.095	8.4	12.96	71
13	4.3820	56.966	19.202	11.0	4.00	62
15	4.4998	67.497	20.248	10.0	25.00	49
19	2.9957	56.918	8.974	22.1	9.61	30
28	2.3026	64.473	5.302	27.7	0.09	10
Σ=97	Σ=33.908	Σ=351.75	Σ=151.10		Σ=111.08	

$a = (n\Sigma xy-\Sigma x\Sigma y)/(n\Sigma x^2-(\Sigma x)^2)$
$= ((8)(351.75)-(33.908)(97))/((8)(151.1)-(33.908)^2)$
$= -8.0457$

$b = (\Sigma x^2\Sigma y-\Sigma xy\Sigma x)/(n\Sigma x^2-(\Sigma x)^2)$
$= ((151.1)(97)-(351.75)(33.908))/((8)(151.1)-(33.908)^2)$
$= 46.227$

$k = (-1/a) = 0.124/hr.$

$So = \exp(-b/a) = 313$ ppm

* $Sc=So*\exp(-kt)$

Monod Kinetics (Constant Biomass)

Two-Parameter Model: $t = (K/k)\ln(So/S)+(1/k)(So-S)$; (refer to A-13)

$y = a\ x + b\ z$

y=t	x=ln(So/S)	z = (So-S)	xy	xz	yz	x^2	z^2
0	0	0	0	0	0	0	0
1	0.0645	10	0.0645	0.645	10	0.0042	100
9	0.1335	20	1.2015	2.670	180	0.0178	400
12	0.3747	50	4.4964	18.735	600	0.1404	2500
13	0.6931	80	9.0103	55.448	1040	0.4804	6400
15	0.5754	70	8.6310	40.278	1050	0.3311	4900
19	2.0794	140	39.5094	291.116	2660	4.3239	19600
28	2.7726	150	77.6325	415.890	4200	7.6873	22500
			Σ=140.55	Σ=824.78	Σ=9740	Σ=12.985	Σ=56400

$a = (\Sigma xy \Sigma z^2 - \Sigma xz \Sigma yz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$
$= ((140.55)(56400)-(824.78)(9740))/((12.985)(56400)-(824.78)^2)$
$= -2.041$

$b = (\Sigma yz \Sigma x^2 - \Sigma xy \Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$
$= ((9740)(12.985)-(140.55)(824.78))/((12.985)(56400)-(824.78)^2)$
$= 0.20255$

$k = (1/b) = (1/0.20255) = 4.94$ ppm/hr.

$K = (a/b) = (-2.041/0.20255) = -10.1$ ppm

yc = tc=ax+bz	(t-tc)^2	Sc*
0	0	160
1.9	0.81	155
3.8	27.04	112
9.4	6.76	96
14.8	3.24	90
13.0	4.00	79
24.1	26.01	56
24.7	10.89	--**
	Σ=78.75	

* by Newton's rule (i.e., trial-and-error procedure) ; (refer to A-23)

f(S) = a*ln(S/So)+b*(S-So)+t=0
= -2.041*ln(S/160)+0.20255*(S-160)+t=0
f'(S) = a/S+b=0
= -2.041/S+0.20255=0

for t = 0 ⟶ let Si=So=160
Sii=Si-f(Si)/f'(Si)
=160-0/0.19=160
|Sii-Si| = 160-160 = 0<1E-1 (convergence value)
therefore S at t=0 is 160 ppm

for t=1 ⟶ let Si=160
Sii=Si-f(Si)/f'(Si)
=160-1/0.19=154.7
|Sii-Si| = 160-154.7 = 5.3>1E-1
let Si=154.7
Sii=154.7-(-0.00476)/(0.189)=154.7
|Sii-Si| = 154.7-154.7 = 0<1E-1
therefore S at t=1 is 154.7 ppm

to determine the remaining values of S at the corresponding values of t, the basic program on A-24 is used.

**the value of Sc at t = 28 is indeterminate due to the negative value of K!

Monod Kinetics (Constant Biomass)

Three-Parameter Model: $t = (-K/k)\ln S+(-1/k)S+((K/k)\ln So+So/k)$
$y = a x + b z+ c$;(refer to A-14)

y=t	x=lnS	z = S	xy	xz	yz	x^2	z^2
0	5.0752	160	0	812.03	0	25.76	25600
1	5.0106	150	5.011	751.59	150	25.51	22500
9	4.9416	140	44.474	691.82	1260	24.42	19600
12	4.7005	110	56.406	517.05	1320	22.10	12100
13	4.3820	80	56.966	350.56	1040	19.20	6400
15	4.4998	90	67.497	404.98	1350	20.25	8100
19	2.9957	20	56.918	59.91	380	8.97	400
28	2.3026	10	64.473	23.03	280	5.30	100
Σ=97	Σ=33.908	Σ=760	Σ=351.75	Σ=3611	Σ=5780	Σ=151.1	Σ=94800

A1 = 151.1 ; B1 = 3611 ; C1 = 33.91 ; D1 = 351.75
A2 = 3611 ; B2 = 94800 ; C2 = 760 ; D2 = 5780 (refer to A-22)
A3 = 33.91 ; B3 = 760 ; C3 = 8 ; D3 = 97

E1 = (3611/151.1) = 23.90 ; F1 = (33.91/151.1) = 0.2244
E2 = (94800/3611) - 23.90 = 2.355 ; F2 = (760/3611) - 0.2244 = -0.01395
E3 = (760/33.91) - 23.90 = -1.486 ; F3 = (8/33.91) - 0.2244 = 0.01150

G1 = (351.75/151.1) = 2.328 ; H1 = 0.2244-23.90* -0.005924 = 0.3660
G2 = (5780/3611) - 2.328 = -0.7273 ; H2 = -0.01395/2.355 = -0.005924
G3 = (97/33.91) - 2.328 = 0.5326 ; H3 = 0.01150/-1.486 - -0.005924 = -0.001815

I1 = 2.328 - 23.90* -0.3088 = 9.709
I2 = -0.7273/2.355 = -0.3088
I3 = 0.5326/-1.486 - -0.3088 = -0.04958

a = 9.709 - -0.04958*0.366/-0.001815 = -0.2890
b = -0.3088 - -0.04958* -0.005924/-0.001815 = -0.1470
c = -0.04958/-0.001815 = 27.32

$\boxed{k = (-1/b) = (-1/-0.1470) = 6.80 \text{ ppm/hr}}$

$\boxed{K = (a/b) = (-0.2890/-0.1470) = 1.97 \text{ ppm}}$

yc = tc = ax + bz + c	(t-tc)^2	Sc*
2.3	5.29	176
3.8	7.84	169
5.3	13.69	115
9.8	4.84	95
14.3	1.69	89
12.8	4.84	75
23.5	20.25	49
25.2	7.84	.03
	Σ= 66.28	

*as per Newton's rule (refer to A-20)

Zero-Order Kinetics (Variable Biomass)

One-Parameter Model: $t = (1/koYc)(\ln(Bo + YcSo - YcS) - \ln(Bo))$; (refer to A-7)

$y = a \quad x$

y=t	x=f(S)*	xy	x^2	yc=tc=ax	(t-tc)^2	Sc=f(t)**
0	0	0	0	0	0	160
1	0.0681	0.0681	0.00464	2.3	1.69	156
9	0.1318	1.1862	0.01737	4.5	20.25	117
12	0.3018	3.6216	0.09108	10.3	1.70	100
13	0.4471	5.8123	0.19990	15.2	4.84	94
15	0.4010	6.0150	0.16080	13.7	1.69	81
19	0.6864	13.0416	0.47114	23.4	19.36	54
28	0.7212	20.1936	0.52013	24.6	11.56	-21
		Σ= 49.9384	Σ= 1.4651		Σ=61.09	

$a = \Sigma xy/\Sigma x^2 = (49.9384)/(1.4651) = 34.1$ hr.

$\boxed{ko = (1/aYc) = 1/((34.1)(0.136)) = 0.216/hr.}$

* f(S) = $(\ln(Bo+YcSo-YcS)-\ln(Bo))$, where Bo = 19.3 ppm and Yc = 0.136

** f(t) = $(Bo+YcSo-Bo*\exp(koYct))/Yc$

First-Order Kinetics (Variable Biomass)

One-Parameter Model: $t = (-1/(ko(Bo+YcSo)))\ln(BoS/((Bo+YcSo-YcS)So))$

$y = a x$; (refer to A-11)

y=t	x=f(S)*	xy	x^2	yc=tc=ax	(t-tc)^2	Sc=f(t)**
0	0	0	0	0	0	160
1	-0.1326	-0.133	0.0176	1.1	0.01	151
9	-0.2654	-2.389	0.0704	2.2	46.24	84
12	-0.6765	-8.118	0.4577	5.7	39.69	64
13	-1.1402	-14.823	1.3001	9.6	11.56	58
15	-0.9763	-14.645	0.9532	8.2	46.24	48
19	-2.7658	-52.550	7.6496	23.3	18.49	32
28	-3.4938	-97.826	12.2066	29.4	1.96	12
		$\Sigma = -190.48$	$\Sigma = 22.655$		$\Sigma = 164.19$	

$a = \Sigma xy/\Sigma x^2 = (-190.48)/(22.655) = -8.408$ hr.

$$\boxed{ko = (-1/(a(Bo+YcSo))) = (-1/(-8.408(19.3 + (0.136)(160)))) = 0.00290/\text{ppm hr.}}$$

* $f(S) = \ln(BoS/((Bo+YcSo-YcS)So))$, where Bo = 19.3 ppm and Yc = 0.136

** $Sc = f(t) = (Bo + YcSo)/(Yc + (Bo/So)\exp((Bo+YcSo)kot))$

Monod Kinetics (Variable Biomass)

Two-Parameter Model: $t = (K/(ko(Bo+YcSo)))\ln(Bo+YcSo-YcS)So/(BoS)) + (1/(koYc))\ln((Bo+YcSo-YcS)/Bo)$

$y = ax+bz$; (refer to A-16)

where,

$a = (K/(ko(Bo+YcSo)))$; Bo = 19.3 ppm and Yc = 0.136

$x = \ln((Bo+YcSo-YcS)So/(BoS))$

$b = (1/(koYc))$

$z = \ln((Bo+YcSo-YcS)/Bo)$

y	x	z	xy	xz	yz	x ^ 2	z^2
0	0	0	0	0	0	0	0
1	0.1326	0.0681	0.1326	0.00903	0.0681	0.01758	0.0046
9	0.2654	0.1318	2.3886	0.03498	1.1862	0.07044	0.0173
12	0.6765	0.3018	8.1180	0.20417	3.6216	0.45765	0.0910
13	1.1402	0.4471	14.8226	0.50978	5.8123	1.30006	0.1999
15	0.9763	0.4010	14.6445	0.39150	6.0150	0.95316	0.1608
19	2.7658	0.6864	52.5502	1.89845	13.0416	7.64965	0.4711
28	3.4938	0.7212	97.8264	2.51973	20.1936	12.20664	0.5201
			Σ=190.48	Σ= 5.5676	Σ=49.938	Σ=22.655	Σ=1.4651

$a = (\Sigma xy\Sigma z^2 - \Sigma xz\Sigma yz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$
$= ((190.48)(1.4651)-(5.5676+(49.938))/((22.655)(1.4651)-(5.5676)^2)$
$= 0.4729$

$b = (\Sigma yz\Sigma x^2 - \Sigma xy\Sigma xz)/(\Sigma x^2 \Sigma z^2 - (\Sigma xz)^2)$
$= ((49.938)(22.655)-(190.48)(5.5676))/((22.655)(1.4651)-(5.5676)^2)$
$= 32.288$

ko = (1/(bYc))
= (1/(32.288*0.136)
= 0.228/hr.

K = (a(Bo+YcSo))/(bYc)
= ko*a(Bo+YcSo)
= 0.228*0.4729*(19.3+0.136*160)
= 4.43 ppm

yc=tc=ax+bz	(t-tc)^2	Sc*
0	0	160
2.3	1.69	156
4.4	21.16	116
10.1	3.61	99
15.0	4.00	93
13.4	2.56	80
23.5	20.25	53
24.9	9.61	.15
	Σ=62.88	

* as per Newton's rule (refer to A-20)

LOTUS 123 Spreadsheets

General Description

Two spreadsheets were created using LOTUS 123 software to facilitate the cumbersome regression calculations demonstrated on the preceding pages of this appendix. The first spreadsheet performs the regression of batch-reactor biodegradation data under the assumption of constant biomass, while the second is for the case in which variable biomass data are available.

The format of the two spreadsheets are identical, as can be seen in the following printouts. The top sheet of each is a summary of inputted data and calculated results. Each subsequent sheet contains the detailed calculations for a given model.

Operation of the spreadsheets involves inputting the following information on the summary sheet: (1) the data reference, (2) the number of data points, and (3) the actual S vs. t data. For the case of variable biomass, Bo and Yc must also be inputted. The LOTUS 123 program automatically calculates all the results except for the values of Scalc for the Monod models. The calculation of Scalc in the case of the Monod models is accomplished on a Sharp PC-1500 (refer to A-24) using the regressed constants from the spreadsheets. The values of Scalc must then be inputted on the spreadsheet (i.e., under the "Scalc" column of the Monod sub-sheets) to complete the analysis.

The spreadsheets, as presented, can handle up to 25 (S vs. t) data points. Minor modifications are necessary to increase the capability, if desired.

It should be noted that, although not presented in this appendix, two spreadsheets analogous to those shown here for batch reactor data analysis were developed and used in this thesis for CSTR data analysis. The only notable difference between the two sets of spreadsheets is in the calculation of S as a function of time (i.e., real time for the batch reactor and residence time for the CSTR). For the case of the CSTR, trial-and-error solution is not required for the Monod equation; S is directly determined through the use of the quadratic formula for all three of the Monod models, as well as for the first-order variable-biomass model. Caution must be applied when using the quadratic formula in these spreadsheets, however, to ensure that the proper sign (i.e., positive or negative) is used. As a further side note, two variations of the variable-biomass spreadsheet were developed depending on the form of the biomass data (i.e., either Bo and Yc for true CSTR operation or Be for the case in which biomass is controlled by recycling/wasting).

gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Klecka,G.M.,et al (data set #4)

n.pts.= 8

Raw Data

(ppm)	t(hr)
160	0
150	1
140	9
110	12
80	13
90	15
20	19
10	28
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.790554	---	160	10.36879	347.6710
(2-parameter)	6.579330	---	174.7743	8.348174	361.3723
First-order					
(1-parameter)	0.092391	---	160	30.47460	1476.580
(2-parameter)	0.124351	---	313.0210	13.91000	5565.808
Monod Kinetics					
(2-parameter)	4.934976	-10.1036	160	9.884875	ERR *
(3-parameter)	6.758245	1.576952	175.4876	8.343651	331.2070

Refer to C-22

Zero-order (1-parameter): t=(1/k)*(So-S) ; (minimization of dt^2)
------------------------- y= a * x ; where y=t
x=(So-S)
a=(1/k)

y=t	x=So-S	x*y	x^2	tc=a*x	(t-tc)^2	Scalc	(S-Sc)^2
0	0	0	0	0	0	160	0
1	10	10	100	1.726950	0.528456	154.2094	17.71943
9	20	180	400	3.453900	30.75921	107.8850	1031.372
12	50	600	2500	8.634751	11.32489	90.51334	379.7296
13	80	1040	6400	13.81560	0.665207	84.72279	22.30477
15	70	1050	4900	12.08865	8.475944	73.14168	284.2028
19	140	2660	19600	24.17730	26.80448	49.97946	898.7683
28	150	4200	22500	25.90425	4.392145	-2.13552	147.2709
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
		9740	56400		82.95035		2781.368

k = 5.790554 ppm/hr

Zero-order (2-parameter): t=(-1/k)S+(So/k) ; (minimization of dt^2)
y= a x+ b ; where y=t
x=S
a=(-1/k)
b=(So/k)

y=t	x=S	x*y	x^2	tc=ax+b	(t-tc)^2	Scalc	(S-Sc)^2
0	160	0	25600	2.245575	5.042608	174.7743	218.2823
1	150	150	22500	3.765486	7.647916	168.1950	331.0598
9	140	1260	19600	5.285398	13.79826	115.5604	597.2936
12	110	1320	12100	9.845132	4.643452	95.82241	201.0038
13	80	1040	6400	14.40486	1.973652	89.24308	85.43463
15	90	1350	8100	12.88495	4.473412	76.08442	193.6432
19	20	380	400	23.52433	20.46961	49.76710	886.0804
28	10	280	100	25.04424	8.736471	-9.44687	378.1807
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
97	760	5780	94800		66.78539		2890.978

k = 6.579330 ppm/hr

So= 174.7743 ppm

First-order (1-parameter): t=(1/k)ln(So/S) ; (minimization of dt^2)
-------------------------- y= a x ; where y=t
x=ln(So/S)
a=(1/k)

y=t	x	x*y	x^2	tc=a*x	(t-tc)^2	Scalc	(S-Sc)^2
0	0	0	0	0	0	160	0
1	0.064538	0.064538	0.004165	0.698534	0.090881	145.8797	16.97658
9	0.133531	1.201782	0.017830	1.445281	57.07377	69.66182	4947.459
12	0.374693	4.496321	0.140395	4.055507	63.11496	52.79827	3272.036
13	0.693147	9.010913	0.480453	7.502301	30.22468	48.13874	1015.139
15	0.575364	8.630462	0.331043	6.227473	76.95722	40.01701	2498.298
19	2.079441	39.50938	4.324077	22.50690	12.29838	27.65315	58.57072
28	2.772588	77.63248	7.687248	30.00920	4.036912	12.03980	4.160806
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
		140.5458	12.98521		243.7968		11812.64

k = 0.092391 /hr

```
First-order (2-parameter): t=(-1/k)lnS+(lnSo)/k ; (minimization of dt^2)
-------------------------- y=    a    x +    b      ; where y=t
                                                            x=lnS
                                                            a=(-1/k)
                                                            b=(lnSo)/k
```

y=t	x=lnS	x*y	x^2	tc=ax+b	(t-tc)^2	Scalc	(S-Sc)^2
0	5.075173	0	25.75738	5.396779	29.12523	313.0210	23415.45
1	5.010635	5.010635	25.10646	5.915781	24.16490	276.4193	15981.86
9	4.941642	44.47478	24.41982	6.470603	6.397846	102.2180	1427.473
12	4.700480	56.40576	22.09451	8.409963	12.88835	70.39023	1568.933
13	4.382026	56.96634	19.20215	10.97088	4.117314	62.15947	318.2842
15	4.499809	67.49714	20.24828	10.02370	24.76352	48.47269	1724.517
19	2.995732	56.91891	8.974411	22.11909	9.728724	29.47655	89.80515
28	2.302585	64.47238	5.301898	27.69319	0.094130	9.625668	0.140124
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
0	0	0	0	NA	0	NA	0
97	33.90808	351.7459	151.1049		111.2800		44526.47

k = 0.124351 /hr

So= 313.0210 ppm

Monod (2-parameter): t=(K/k)*ln(So/S)+(1/k)*(So-S) ; (minimization of dt^2)

y= a * x + b * z ; where y=ln(So/S)

z=(So-S)

a=(K/k)

b=(1/k)

y=t	x	z	x*y	y*z	x*z	x^2	z^2	tc=ax+bz	(t-tc)^2	Scalc	(S-Sc)^2
0	0	0	0	0	0	0	0	0	0	160	0
1	0.064538	10	0.064538	10	0.645385	0.004165	100	1.894219	0.799628	154.7264	22.33885
9	0.133531	20	1.201782	180	2.670627	0.017830	400	3.779319	27.25550	111.9797	785.1372
12	0.374693	50	4.496321	600	18.73467	0.140395	2500	9.364633	6.945155	95.5742	208.1037
13	0.693147	80	9.010913	1040	55.45177	0.480453	6400	14.79170	3.210207	90.0361	100.7233
15	0.575364	70	8.630462	1050	40.27549	0.331043	4900	13.00649	3.974059	78.8222	124.9432
19	2.079441	140	39.50938	2660	291.1218	4.324077	19600	24.11159	26.12840	55.5463	1263.539
28	2.772588	150	77.63248	4200	415.8883	7.687248	22500	24.71883	10.76604	ERR	ERR
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
			140.5458	9740	824.7880	12.98521	56400		79.07900		ERR

k = 4.934976 ppm/hr

K = -10.1036 ppm

* The value of Scalc at t = 28 is indeterminate due to the negative value of K !!!

Monod (3-parameter): t=(-K/k)*lnS+(-1/k)*S+((K/k)*lnSo+(So/k)) ; (minimization of dt^2)

y= a * x + b *z+ c ; where y=t
x=lnS
z=S
a=(-K/k)
b=(-1/k)
c=((K/k)lnSo+(So/k))

y=t	x	z	x*y	y*z	x*z	x^2	z^2	tcalc	(t-tc)^2	Scalc	(S-Sc)^2
0	5.075173	160	0	0	812.0278	25.75738	25600	2.311894	5.344858	175.4876	239.8657
1	5.010635	150	5.010635	150	751.5952	25.10646	22500	3.806628	7.877161	168.7904	353.0791
9	4.941642	140	44.47478	1260	691.8299	24.41982	19600	5.302400	13.67224	115.3225	608.9790
12	4.700480	110	56.40576	1320	517.0528	22.09451	12100	9.797694	4.850150	95.3467	214.7192
13	4.382026	80	56.96634	1040	350.5621	19.20215	6400	14.31102	1.718781	88.702	75.72480
15	4.499809	90	67.49714	1350	404.9828	20.24828	8100	12.80386	4.823004	75.4402	211.9877
19	2.995732	20	56.91891	380	59.91464	8.974411	400	23.51254	20.36302	49.0837	845.8616
28	2.302585	10	64.47238	280	23.02585	5.301898	100	25.15395	8.099989	0.0281	99.43878
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
0	0	0	0	0	0	0	0	27.17090	0	NA	0
97	33.90808	760	351.7459	5780	3610.991	151.1049	94800		66.74921		2649.656

A1=151.1049	B1=3610.991	C1=33.90808	D1=351.7459
A2=3610.991	B2= 94800	C2= 760	D2= 5780
A3=33.90808	B3= 760	C3= 8	D3= 97

E1=23.89724	F1=0.224400	G1=2.327825
E2=2.355938	F2=-0.01393	G2=-0.72715
E3=-1.48370	F3=0.011531	G3=0.532849

H1=0.365722	I1=9.703675
H2=-0.00591	I2=-0.30864
H3=-0.00185	I3=-0.05048

a=-0.23333
b=-0.14796
c=27.17090

k = 6.758245 ppm/hr

K = 1.576952 ppm

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #4)

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
160	0
150	1
140	9
110	12
80	13
90	15
20	19
10	28
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 19.3 ppm
Yc = 0.136

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.215716	---	7.845138	379.4158
First-order (1-parameter)	0.002896	---	20.42922	946.3390
Monod Kinetics (2-parameter)	0.227597	4.375302	7.804136	268.9583

Zero-order (1-parameter): t=(1/koYc)*ln((Bo+YcSo-YcS)/Bo);(min. of dt^2)
------------------------- y= a * x ;

where y=t
x=ln(Bo+YcSo-YcS)/Bo
a=(1/koYc)

y=t	x	x*y	x^2	tc=a*x	(t-tc)^2	Scalc	(S-Sc)^2
0	0	0	0	0	0	160	0
1	0.068094	0.068094	0.004636	2.321071	1.745230	155.7749	33.35057
9	0.131846	1.186614	0.017383	4.494117	20.30297	117.1175	523.6052
12	0.301830	3.621962	0.091101	10.28821	2.930204	100.1162	97.68943
13	0.447074	5.811966	0.199875	15.23902	5.013223	94.10833	199.0451
15	0.400964	6.014467	0.160772	13.66731	1.776043	81.55067	71.39109
19	0.686388	13.04138	0.471129	23.39631	19.32758	54.11289	1163.689
28	0.721246	20.19489	0.520195	24.58446	11.66585	-20.7661	946.5550
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
		49.93938	1.465095		62.76110		3035.326

a = 34.08610 ko = 0.215716 /hr

First-order (1-parameter): t=-1/(ko(Bo+YcSo))*ln(BoS/((Bo+YcSo-YcS)So))
-------------------------- y= a x

where y=t
x=ln(BoS/((Bo+YcSo-YcS)So))
a=(-1/(ko(Bo+YcSo)))

y=t	x	x*y	x^2	tc=a*x	(t-tc)^2	Scalc	(S-Sc)^2
0	0	0	0	0	0	160	0
1	-0.13263	-0.13263	0.017591	1.115153	0.013260	151.0337	1.068607
9	-0.26537	-2.38839	0.070425	2.231246	45.81602	84.17046	3116.936
12	-0.67652	-8.11828	0.457684	5.688090	39.84020	64.29009	2089.394
13	-1.14022	-14.8228	1.300105	9.586779	11.65007	58.47721	463.2303
15	-0.97632	-14.6449	0.953217	8.208797	46.12043	48.06871	1758.233
19	-2.76583	-52.5507	7.649816	23.25460	18.10168	31.78683	138.9295
28	-3.49383	-97.8273	12.20688	29.37554	1.892110	11.70852	2.919067
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
NA	NA	0	0	NA	0	NA	0
		-190.485	22.65572		163.4337		7570.712

a = -8.40782

ko = 0.002896 /ppm-hr

Monod (2-parameter): (minimization of dt^2)

```
t=(K/(ko(Bo+YcSo)))*ln((Bo+YcSo-YcS)So/(BoS))+(1/(koYc))*ln((Bo+YcSo-YcS)/Bo)
y=       a       *           x              +    b    *         z

where , y=t
        x=ln((Bo+YcSo-YcS)So/(BoS))
        z=ln((Bo+YcSo-YcS)/Bo)
        a=(K/(ko(Bo+YcSo)))
        b=(1/(koYc))
```

y=t	x	z	x*y	y*z	x*z	x^2	z^2	tc=ax+bz	(t-tc)^2	Scalc	(S-Sc)^2
0	0	0	0	0	0	0	0	0	0	160	0
1	0.132632	0.068094	0.132632	0.068094	0.009031	0.017591	0.004636	2.262011	1.592672	155.6608	32.04465
9	0.265377	0.131846	2.388396	1.186614	0.034988	0.070425	0.017383	4.383775	21.30952	116.0111	575.4673
12	0.676523	0.301830	8.118284	3.621962	0.204195	0.457684	0.091101	10.06792	3.732924	98.6628	128.5321
13	1.140221	0.447074	14.82287	5.811966	0.509763	1.300105	0.199875	14.97740	3.910111	92.557	157.6782
15	0.976328	0.400964	14.64492	6.014467	0.391473	0.953217	0.160772	13.41100	2.524910	79.8527	102.9676
19	2.765830	0.686388	52.55077	13.04138	1.898434	7.649816	0.471129	23.46998	19.98074	52.5253	1057.895
28	3.493834	0.721246	97.82737	20.19489	2.519914	12.20688	0.520195	24.93696	9.382204	0.147	97.08160
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
NA	NA	NA	0	0	0	0	0	NA	0	NA	0
			190.4852	49.93938	5.567801	22.65572	1.465095		62.43309		2151.666

a = 0.468190   ko = 0.227597 /hr

b = 32.30683   K = 4.375302 ppm

Appendix D

Compilation of Regression Analysis Results for Aerobic Biodegradation Data from Literature Sources

Table of Contents

Literature References

1. Allard, A-S., Remberger, M. and Neilson, A.H., "Bacterial O-Methylation of Chloroguaiacols: Effect of Substrate Concentration, Cell Density, and Growth Conditions," Applied and Environmental Microbiology, February 1985, pp. 279-288.

2. Beltrame, P., Beltrame, P.L. and Carniti, P., "Influence of Feed Concentration on the Kinetics of Biodegradation of Phenol in a Continuous Stirred Reactor," Water Research, Vol. 18, pp. 403-407 (1984).

3. Beltrame, P., Beltrame, P.L., Carniti, P. and Pitea, D., "Kinetics of Biodegradation of Mixtures Containing 2,4-Dichlorophenol in a Continuous Stirred Reactor," Water Research, Vol. 16, pp. 429-433 (1982).

4. Blanchard, F.A., Takahashi, I.T. and Alexander, H.C., "Biodegradability of [^{14}C] Methylcellulose by Activated Sludge," Applied and Environmental Mirobiology, Vol. 32, No. 4, pp. 557-560 (1976).

5. Cech, J.S. and Chudoba, J., "Influence of Accumulation Capacity of Activated Sludge on Kinetics of Glucose Removal," Water Research, Vol. 17, No. 6, pp. 659-666 (1983).

6. Chudoba, J., Grau, P. and Ottova, V., "Control of Activated-Sludge Filamentous Bulking-II. Selection of Microorganisms by Means of a Selector," Water Research, Vol. 7, pp. 1389-1406 (1973).

7. Garbara, S.V. and Rotmistrov, M.N., "Biodegradation of Hexamethylenediamine by Bacillus subtilis in a Medium with Clay Minerals," Microbiology, 51, pp. 279-281 (1982).

8. Hill, G.A. and Robinson, C.W., "Substrate Inhibition Kinetics: Phenol Degradation by Pseudomonas putida," Biotechnology and Bioengineering, Vol. XVII, pp. 1599-1615 (1975).

9. Ilyalendinov, A.N., Alieva, R.M. and Dzhusupova, D.E., "Bacteria that Decompose α-Methylstyrene," Microbiology, 2, pp. 477-481 (1983).

10. Kaplan, D.L. and Kaplan, A.M., "Biodegradation of N-Nitrosodimethylamine in Aqueous and Soil Systems," Applied and Environmental Microbiology, Vol. 50, No. 4, pp. 1077-1086 (1985).

11. Klecka, G.M. and Maier, W.J. , "Kinetics of Microbial Growth on Pentachlorophenol," Applied and Environmental Microbiology, Vol. 49, No. 1, pp. 46-53 (1985).

12. Larson, R.J., Games, L.M. and King, J.E., "Fate and Distribution of a Quaternary Ammonium Surfactant, Octadecyltrimethylammonium Chloride (OTAC), in Wastewater Treatment," Environmental Science Technology, Vol. 16, No. 8, pp. 483-488 (1982).

13. Liu, D., Strachan, W.M.J., Thomson, K. and Kwasniewska, K., "Determination of the Biodegradability of Organic Compounds," Environmental Science and Technology, Vol. 15, No. 7, pp. 788-792 (1981).

14. Lyons, C.D., Katz, S. and Bartha, R., "Mechanisms and Pathways of Aniline Elimination from Aquatic Environments," Applied and Environmental Microbiology, Vol. 48, No. 3, pp. 491-496 (1984).

15. Papanastasiou, A.C. and Maier, W.J., "Kinetics of Biodegradation of 2,4-Dichlorophenoxyacetate in the Presence of Glucose," Biotechnology and Bioengineering, Vol. XXIV, pp. 2001-2011 (1982).

16. Radhakrishnan, I. and Sinha Ray, A.K., "Activated Sludge Studies with Phenol Bacteria," Journal WPCF, Vol. 46, No. 10, pp. 2393-2418 (1974).

17. Saeger, V.W. and Tucker, E.S., "Biodegradation of Phthalic Acid Esters in River Water and Activated Sludge," Applied and Environmental Microbiology, Vol. 31, No. 1, pp. 29-34 (1976).

18. Sayler, G.S., Breen, A., Blackburn, J.W. and Yagi, O., "Predictive Assessment of Priority Pollutant Bio-oxidation Kinetics in Activated Sludge," Environmental Progress, Vol. 3, No. 3, pp. 153-163 (1984).

19. Shamat, N.A. and Maier, W.J., "Kinetics of Biodegradation of Chlorinated Organics," Journal WPCF, Vol. 52, No. 8, pp. 2158-2166 (1980).

20. Tanner, R.D., "An Enzyme Kinetic Model for Describing Fermentation Processes," Biotechnology and Bioengineering, Vol. XII, pp. 831-843 (1970).

21. Taylor, B.F. and Ribbons, D.W., "Bacterial Decarboxylation of o-Phthalic Acids," Applied and Environmental Microbiology, Vol. 46, No. 6, pp. 1276-1281 (1983).

22. Wong, P.T.S. and Kaiser, K.L.E., "Bacterial Degradation of Polychlorinated Biphenyls II. Rate Studies," Bulletin of Environmental Contamination and Toxicology, Vol. 13, No. 2 (1975).

23. Wong, P.T.S., Liu, D., and Dutka, B.J., "Rapid Biodegradation of NTA by a Novel Bacterial Mutant," Water Research, 6, pp. 1577-1584 (1972).

24. Yordy, J.R. and Alexander, M., "Microbial Metabolism of N-Nitrosodiethanolamine in Lake Water and Sewage," Applied and Environmental Microbiology, Vol. 39, No. 3, pp. 559-565 (1980).

Index of Batch Reactor Data Analysis Results

Reference	Substrate	Medium	Biomass Type	# Sets	Page
16	Phenol	B.Cereus	Constant	3	D-59,D-61, D-63
			Variable	3	D-60,D-62, D-64
17	Butyl benzyl phthalate	Activated sludge	Constant	1	D-68
	Butylglycolyl butyl phthalate	Activated sludge	Constant	1	D-69
18	Phenol	Activated sludge	Constant	2	D-70,D-71
19	3,5-dichlorobenzoate	Activated sludge	Constant	1	D-72
			Variable	1	D-73
20	Glucose	P.ovalis	Constant	1	D-74
			Variable	1	D-75
21	o-phthalic acid	Activated sludge	Constant	3	D-76 to D-78
22	4-chlorobiphenyl	Lake water	Constant	1	D-79
	2-chlorobiphenyl	Lake water	Constant	1	D-80
	Biphenyl	Lake water	Constant	1	D-81
23	Nitrilotriacetic acid	Bacterial mutant	Constant	1	D-82
			Variable	1	D-83
24	N-nitrosodiethanolamine	Lake water	Constant	5	D-84 to D-88
		Activated sludge	Constant	1	D-89

Index of CSTR Data Analysis Results

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Allard,A-C.,et al (data set #1) ;

Substrate : 3,4,5-trichloroguaiacol
Culture : strain 1395

Num.pts.= 14

Raw Data

S(ppm)	t(hr)
13.8	0
13.5	12
13.7	24
13.6	36
13.6	48
12.5	72
12	96
12.1	120
11.5	144
10.3	168
10	192
10.3	216
9.5	240
8.3	264
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.018760	---	13.8	429.9616	0.151330
(2-parameter)	0.020853	---	14.19520	277.1787	0.120535
First-order					
(1-parameter)	0.001630	---	13.8	669.0595	0.222786
(2-parameter)	0.001875	---	14.46674	381.5715	0.171876
Monod Kinetics					
(2-parameter)	0.007780	-6.78483	13.8	304.8192	0.112526
(3-parameter)	0.010604	-5.52034	14.0431	243.7066	0.106820

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Allard,A-C.,et al (data set #2) ;

Substrate : 3,4,5-trichloroguaiacol
Culture : strain 1395

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
1.31	0
1.12	12
0.95	24
0.68	48
0.45	72
0.33	96
0.23	120
0.15	144
0.1	168
0.06	192
0.03	216
0.02	240
0.01	264
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.006854	---	1.31	1487.169	0.069881
(2-parameter)	0.005548	---	1.099703	1210.912	0.037285
First-order					
(1-parameter)	0.016925	---	1.31	153.1641	0.002519
(2-parameter)	0.018134	---	1.645657	93.93489	0.013272
Monod Kinetics					
(2-parameter)	0.028253	1.298568	1.31	18.90113	0.000630
(3-parameter)	0.024477	1.105226	1.259	16.46033	0.000585

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Allard,A-C.,et al (data set #3) ;

Substrate : 3,4,5-trichloroguaiacol
Culture : strain 1395

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
0.125	0
0.103	8
0.093	12
0.073	24
0.055	32
0.013	40
0.005	48
0.001	72
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.002215	---	0.125	52.06004	0.000255
(2-parameter)	0.002134	---	0.121461	51.20181	0.000233
First-order					
(1-parameter)	0.062617	---	0.125	90.48412	0.000675
(2-parameter)	0.076922	---	0.264460	39.54942	0.002902
Monod Kinetics					
(2-parameter)	0.003544	0.023061	0.125	25.08831	0.000079
(3-parameter)	0.004623	0.035382	0.1377	22.13866	0.000106

Regression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Beltrame,P.,et al,1984 (data set #1) ; Substrate : phenol
Culture : activated sludge
Condition : 20C & pH 7.4

Num.pts.= 7

Raw Data

Se(ppm)	t(hr)*
180	0
120.6	2.5
95.1	3
52.7	3
52.6	3
41.5	4
40.1	4
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

REFERS TO RESIDENCE TIME (V/Q)

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	35.91857	---	180	0.249719	322.1746
(2-parameter)	41.57272	---	199.0383	0.207805	359.1487
First-order					
(1-parameter)	0.788382	---	180	1.035585	764.0452
(2-parameter)	-2.01871	---	-290.572	0.490125	32183.28
Monod Kinetics					
(2-parameter)	27.56509	-11.3995	180	0.202057	ERR
(3-parameter)	31.77148	-8.95707	189.8336	0.188534	ERR

Regression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

Data source -- Beltrame,P.,et al,1984 (data set #1) ; Substrate : phenol
Culture : activated sludge
Condition : 20C & pH 7.4

Num.pts.= 7

Raw Data

Se(ppm)	Be(ppm)	t(hr)*
180	0	0
120.6	393	2.5
95.1	518	3
52.7	1024	3
52.6	1010	3
41.5	968	4
40.1	995	4
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA

Summary of results:

Kinetic Model	ko	K	Si	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.044023	---	180	0.379326	414.2918
First-order (1-parameter)	0.000794	---	180	0.261224	87.09340
Monod Kinetics (2-parameter)	0.093480	66.35367	180	0.000543	0.170120

* REFERS TO RESIDENCE TIME (V/Q)

Regression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Beltrame,P.,et al,1984 (data set #2) ; Substrate : phenol
Culture : activated sludge
Condition : 20C & pH 7.4

Num.pts.= 5

Raw Data

Se(ppm)	t(hr)*
360	0
242	2.5
103	6
72.9	6
53.2	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	47.50123	---	360	0.112063	252.8555
(2-parameter)	48.16284	---	363.6876	0.110491	256.3026
First-order					
(1-parameter)	0.742140	---	360	2.794216	3003.364
(2-parameter)	-1.51579	---	-530.674	1.683140	159517.6
Monod Kinetics					
(2-parameter)	39.97546	-11.2933	360	0.036331	304.4332
(3-parameter)	38.66961	-12.0654	354.7613	0.032327	314.0058

* REFERS TO RESIDENCE TIME (V/Q)

Regression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

Data source -- Beltrame,P.,et al,1984 (data set #2) ; Substrate : phenol
Culture : activated sludge
Condition : 20C & pH 7.4

Num.pts.= 5

Raw Data

Se(ppm)	Be(ppm)	t(hr)*
360	0	0
242	701	2.5
103	828	6
72.9	1114	6
53.2	1484	6
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA

* REFERS TO RESIDENCE TIME (V/Q)

Summary of results:

Kinetic Model	ko	K	Si	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.046122	---	360	0.865433	2679.275
First-order (1-parameter)	0.000577	---	360	0.567228	821.9854
Monod Kinetics (2-parameter)	0.099715	98.20042	360	0.007373	6.910976

Regression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Beltrame,P.,et al,1982 (data set #1) ; Substrate : 2,4-dichlorophenol
Culture : mlss
Condition : 20C & pH 7.9

Num.pts.= 9

Raw Data

Se(ppm)	t(hr)*
156	0
102.1	6.25
104.7	6.25
119	6.25
119.6	6.25
79.4	12.5
92.7	12.5
52.4	25
121.3	25
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.751658	---	156	43.12910	973.7799
(2-parameter)	5.499220	---	166.3468	42.32106	1279.849
First-order					
(1-parameter)	0.069761	---	156	51.79715	506.9556
(2-parameter)	0.225719	---	338.6448	39.96494	4672.997
Monod Kinetics					
(2-parameter)	5.763809	15.68271	156	42.67380	730.4580
(3-parameter)	30.32550	173.0599	220.3071	39.85953	1350.695

* REFERS TO RESIDENCE TIME (V/Q)

Regression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

Data source -- Beltrame,P.,et al,1982 (data set #1) ; Substrate : 2,4-dichlorophenol
Culture : activated sludge
Condition : 20C & pH 7.9

Num.pts.= 9

Raw Data

Se(ppm)	Be(ppm)	t(hr)*
156	0	0
102.1	299	6.25
104.7	257	6.25
119	209	6.25
119.6	208	6.25
79.4	237	12.5
92.7	185	12.5
52.4	208	25
121.3	46	25
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA

* REFERS TO RESIDENCE TIME (V/Q)

Summary of results:

Kinetic Model	ko	K	Si	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.026536	---	156	5.892176	145.6491
First-order (1-parameter)	0.000320	---	156	6.676141	32.83334
Monod Kinetics (2-parameter)	0.049828	77.86616	156	0.120116	3.841822

Regression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Beltrame,P.,et al,1982 (data set #2) ; Substrate : phenol
Culture : mlss
Condition : 20C & pH 7.9

Num.pts.= 9

Raw Data

Se(ppm)	t(hr)*
90	0
31	6.25
32.8	6.25
41.2	6.25
42.9	6.25
23.1	12.5
26.8	12.5
14.9	25
45.7	25
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.619440	---	90	48.17293	1027.973
(2-parameter)	4.641278	---	90.28087	48.17243	1037.705
First-order					
(1-parameter)	0.195922	---	90	47.50346	121.2057
(2-parameter)	-3.04671	---	-1015.91	42.01663	136190.3
Monod Kinetics					
(2-parameter)	9.214093	25.12215	90	42.74211	228.8289
(3-parameter)	24.13884	51.86840	134.0115	41.77610	506.8091

* REFERS TO RESIDENCE TIME (V/Q)

Regression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

Data source -- Beltrame,P.,et al,1982 (data set #2) ; Substrate : phenol
Culture : activated sludge
Condition : 20C & pH 7.9

Num.pts.= 9

Raw Data

Se(ppm)	Be(ppm)	t(hr)*
90	0	0
31	299	6.25
32.8	257	6.25
41.2	209	6.25
42.9	208	6.25
23.1	237	12.5
26.8	185	12.5
14.9	208	25
45.7	46	25
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA

* REFERS TO RESIDENCE TIME (V/Q)

Summary of results:

Kinetic Model	ko	K	Si	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.031216	---	90	25.81877	952.3909
First-order (1-parameter)	0.000933	---	90	1.137048	3.103272
Monod Kinetics (2-parameter)	0.200896	186.8669	90	0.430066	2.929465

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Blanchard,F.A.,et al (data set #1) ; Substrate : methylcellulose
Culture : activated sludge

Num.pts.= 18

Raw Data

S(ppm)	t(hr)
13.5	0
13.2	24
12.3	48
11.1	72
9.9	96
8.9	120
7.3	144
4.7	168
3.4	192
2.9	216
2.1	240
1.8	264
1.8	288
2.4	312
2.6	336
2.7	360
3.1	408
2.7	480
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.036361	---	13.5	4631.659	6.123934
(2-parameter)	0.036718	---	13.59741	4629.990	6.242213
First-order					
(1-parameter)	0.005516	---	13.5	5683.981	1.889516
(2-parameter)	0.006411	---	17.40915	5202.202	2.213958
Monod Kinetics					
(2-parameter)	0.034895	-0.27057	13.5	4629.916	ERR
(3-parameter)	0.035577	-0.18569	13.5615	4629.414	ERR

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Blanchard,F.A.,et al (data set #1);

Substrate : methylcellulose
Culture : activated sludge

Num.pts.= 18

Raw Data

B(ppm)	t(hr)
13.5	0
13.2	24
12.3	48
11.1	72
9.9	96
8.9	120
7.3	144
4.7	168
3.4	192
2.9	216
2.1	240
1.8	264
1.8	288
2.4	312
2.6	336
2.7	360
3.1	408
2.7	480
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 15.2 ppm
Yo = -0.53

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.002988	---	4652.321	3.517327
First-order (1-parameter)	0.000491	---	6403.691	2.571533
Monod Kinetics (2-parameter)	0.002258	-1.52135	4539.146	ERR

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Cech,J.S.,et al (data set #1); Substrate : glucose (measured as COD)
Culture : activated sludge
Condition : 20C & pH 7-8

Num.pts.= 16

Raw Data

S(ppm)	t(hr)
970	0
790	0.25
702	0.5
648	0.75
584	1
540	1.25
520	1.5
490	1.75
460	2
422	2.5
355	3
308	3.5
260	4
205	4.5
160	5
69	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	195.1849	---	970	0.540649	20597.20
(2-parameter)	138.0876	---	791.3305	0.243352	4640.292
First-order					
(1-parameter)	0.382107	---	970	0.150525	2961.212
(2-parameter)	0.379627	---	961.4036	0.150336	2695.288
Monod Kinetics					
(2-parameter)	1086.519	2362.418	970	0.132317	4249.814
(3-parameter)	340.3791	563.4661	841.4649	0.087391	2205.617

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Cech,J.S.,et al (data set #1); Substrate : glucose (measured as COD)
Culture : activated sludge
Condition : 20C & pH 7-8

Num.pts.= 16

Raw Data

S(ppm)	t(hr)
970	0
790	0.25
702	0.5
648	0.75
584	1
540	1.25
520	1.5
490	1.75
460	2
422	2.5
355	3
308	3.5
260	4
205	4.5
160	5
69	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 416 ppm
Yc = 0.811

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.312819	---	0.971500	101226.8
First-order (1-parameter)	0.000513	---	0.233862	9499.275
Monod Kinetics (2-parameter)	-0.60848	-1754.32	0.142632	4053.421

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Chudoba,J.,et al (data set #1) ;

Substrate : peptone/starch @ 1:1 (measured as COD)
Culture : activated sludge

im.pts.= 11

Raw Data

S(ppm)	t(hr)
528	0
283.5	0.25
200.8	0.5
137	0.75
107.5	1
97.8	1.25
78.2	1.75
68.5	2
66.6	2.25
68.5	2.5
58.7	3
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	256.6476	---	528	0.400542	26382.96
(2-parameter)	187.4377	---	413.9568	0.357649	12565.28
First-order					
(1-parameter)	1.016755	---	528	0.196527	4828.483
(2-parameter)	0.785329	---	350.7040	0.151274	3740.073
Monod Kinetics					
(2-parameter)	-143.641	-381.411	528	0.058422	682.6067
(3-parameter)	-131.867	-360.680	468.2589	0.056928	1006.272

gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Garbara,S.V.,et al (data set #1) ;

Substrate : hexamethylenediamine
Culture : Bacillus subtilis
Condition : 20C & pH 5.75-7

m.pts.= 8

Raw Data

S(ppm)	t(hr)
250	0
140	18
125	24
80	36
55	42
30	48
20	60
15	72
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.146854	---	250	55.21872	949.5635
(2-parameter)	3.615737	---	224.9651	46.67348	610.1886
First-order					
(1-parameter)	0.039480	---	250	20.70707	199.1019
(2-parameter)	0.043542	---	308.2977	13.72188	503.2669
Monod Kinetics					
(2-parameter)	12.30052	210.3435	250	9.524709	38.46686
(3-parameter)	13.51403	236.1372	255.205	9.447468	42.44555

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Garbara,S.V.,et al (data set #2) ;

Substrate : hexamethylenediamine
Culture : Bacillus subtilis (w/montmorillonite)
Condition : 20C & pH 7.3-7.45

um.pts.= 5

Raw Data

S(ppm)	t(hr)
250	0
125	18
60	24
25	36
8	42
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	6.417564	---	250	10.58200	435.8212
(2-parameter)	6.122613	---	240.5427	10.00953	375.2212
First-order					
(1-parameter)	0.071727	---	250	27.47603	690.8996
(2-parameter)	0.085396	---	402.6225	15.92470	4977.626
Monod Kinetics					
(2-parameter)	9.946553	51.78108	250	2.347346	75.77945
(3-parameter)	10.27608	54.70523	253.4305	2.311921	75.79461

tegression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Garbara,S.V.,et al (data set #3) ;

Substrate : hexamethylenediamine
Culture : Bacillus subtilis (w/polygorshite)
Condition : 20C & pH 7.45-7.7

um.pts.= 5

Raw Data

S(ppm)	t(hr)
250	0
125	18
55	24
25	36
1	42
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	6.523697	---	250	10.60263	451.2334
(2-parameter)	6.248258	---	241.1582	10.11864	395.0391
First-order					
(1-parameter)	0.106051	---	250	106.2774	1873.965
(2-parameter)	0.150058	---	1232.262	52.25290	193492.5
Monod Kinetics					
(2-parameter)	7.944626	15.92063	250	4.627439	145.4808
(3-parameter)	7.928951	15.85424	249.7057	4.627091	145.4540

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Garbara,S.V.,et al (data set #4) ;

Substrate : hexamethylenediamine
Culture : Bacillus subtilis (w/vermicalite)
Condition : 20C & pH 7.35-7.5

um.pts.= 6

Raw Data

S(ppm)	t(hr)
250	0
125	18
75	24
30	36
10	42
2	48
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.879793	---	250	13.52157	467.4673
(2-parameter)	5.462484	---	234.9495	11.94438	356.4052
First-order					
(1-parameter)	0.082738	---	250	67.71998	1112.371
(2-parameter)	0.107870	---	686.1384	33.11535	31955.92
Monod Kinetics					
(2-parameter)	8.265020	31.71929	250	0.912090	23.19863
(3-parameter)	8.157993	31.00082	248.3	0.901902	23.37671

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Garbara,S.V.,et al (data set #5) ;

Substrate : hexamethylenediamine
Culture : Bacillus subtilis (w/ gintonite)
Condition : 20C & pH 7.3-7.5

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
250	0
125	18
75	24
20	36
1	42
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	6.397927	---	250	4.620034	189.1140
(2-parameter)	6.127972	---	241.2713	4.119167	154.6831
First-order					
(1-parameter)	0.106523	---	250	108.2084	2219.489
(2-parameter)	0.151494	---	1297.839	50.26919	220289.7
Monod Kinetics					
(2-parameter)	7.506017	12.38762	250	0.646405	20.06886
(3-parameter)	7.440827	12.11044	248.7543	0.639556	20.13649

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Hill,G.A.,et al (data set #1); Substrate : phenol
Culture : pseudomonas putida
Condition : 22C & pH 6.2-6.7

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
185	0
156	11.4
144	13.5
138	14.8
106	15.9
94	16.4
59	17.3
31	17.9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	6.351596	---	185	26.76182	1079.646
(2-parameter)	11.19442	---	264.1303	10.91806	1368.199
First-order					
(1-parameter)	0.066898	---	185	57.05012	2231.866
(2-parameter)	0.154241	---	794.3513	16.55234	47460.82
Monod Kinetics					
(2-parameter)	2.555088	-63.5240	185	8.721299	1032.163
(3-parameter)	3.582187	-60.9951	205.8265	5.450662	869.5587

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Hill,G.A.,et al (data set #1); Substrate : phenol
Culture : pseudomonas putida
Condition : 22C & pH 6.2-6.7

Num.pts.= 9

Raw Data

S(ppm)	t(hr)
185	0
156	11.4
144	13.5
138	14.8
106	15.9
94	16.4
59	17.3
31	17.9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 14.3 ppm
Yc = 0.52

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.170988	---	6.240491	565.7221
First-order (1-parameter)	0.001352	---	20.31234	1004.337
Monod Kinetics (2-parameter)	0.086218	-65.7635	1.506825	796.8413

gression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Hill,G.A.,et al (data set #2); Substrate : phenol
Culture : pseudomonas putida
Condition : 22C & pH 6.2-6.7

n.pts.= 7

Raw Data

e(ppm)	t(hr)*
185	0
0.026	3
0.072	3.5
0.218	4.2
0.02	5.5
0.028	6.4
0.071	12
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	32.06774	---	185	7.795110	8016.026
(2-parameter)	32.06411	---	184.9790	7.795110	8014.210
First-order					
(1-parameter)	1224.905	---	185	17.83827	0.005436
(2-parameter)	-0.24383	---	-0.00916	11.43269	4889.777
Monod Kinetics					
(2-parameter)	28.15649	-0.00466	185	7.584023	3273.173
(3-parameter)	28.14988	-0.00466	184.9565	7.584023	3271.637

REFERS TO RESIDENCE TIME (V/Q)

ression of CSTR Biodegradation Data (with respect to time) : Variable Biomass Assumed

a source -- Hill,G.A.,et al (data set #2) ; Substrate : phenol
Culture : pseudomonas putida
Condition : 22C & pH 6.2-6.7

.pts.= 7

Raw Data

(ppm)	Be(ppm)	t(hr)*
185	0	0
0.026	91	3
0.072	87	3.5
0.218	99	4.2
0.02	94	5.5
0.028	99	6.4
0.071	105	12
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA
NA	NA	NA

EFERS TO RESIDENCE TIME (V/Q)

Summary of results:

Kinetic Model	ko	K	Si	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.346120	---	185	9.351193	11498.66
First-order (1-parameter)	13.29875	---	185	18.68579	0.005579
Monod Kinetics (2-parameter)	0.302433	-0.00475	185	9.142830	3343.692

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Ilyalendimov,A.N.,et al (data set #1) ; Substrate : alpha-methylstyrene
Culture : Bacillus cereus
Condition : room temperature/neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
2000	0
1250	28
660	54
400	78
300	101
120	120
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	18.42930	---	2000	164.8791	55999.43
(2-parameter)	16.47227	---	1834.322	142.2816	38606.11
First-order					
(1-parameter)	0.021372	---	2000	55.50385	4995.675
(2-parameter)	0.022794	---	2279.991	44.55066	14447.44
Monod Kinetics					
(2-parameter)	56.46272	1810.713	2000	24.22035	2126.138
(3-parameter)	53.21795	1683.649	1973.7	24.05848	2234.208

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Ilyalendinov,A.N.,et al (data set #2) ; Substrate : alpha-methylstyrene
Culture : P.aeruginosa
Condition : room temperature/neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
2000	0
1100	28
450	54
250	78
130	94
50	117
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	20.90524	---	2000	208.0612	90928.82
(2-parameter)	18.60389	---	1813.674	186.9690	64710.87
First-order					
(1-parameter)	0.029520	---	2000	32.42824	9200.294
(2-parameter)	0.031692	---	2429.313	19.93030	32757.65
Monod Kinetics					
(2-parameter)	75.16183	1874.572	2000	4.303016	856.9466
(3-parameter)	75.87312	1894.904	2005.9	4.299789	848.5866

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Ilyalendinov,A.N.,et al (data set #3) ; Substrate : alpha-methylstyrene
Culture : B.cereus & P.aeruginosa
Condition : room temperature/neutral pH

Num.pts.= 4

Raw Data

S(ppm)	t(hr)
2000	0
1200	24
250	52
30	70
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	30.56590	---	2000	15.77794	14740.93
(2-parameter)	29.78585	---	1957.183	15.10334	13399.63
First-order					
(1-parameter)	0.053629	---	2000	113.3735	109036.1
(2-parameter)	0.064229	---	3819.227	64.54738	867294.2
Monod Kinetics					
(2-parameter)	40.97134	209.5259	2000	1.368673	1284.892
(3-parameter)	42.40001	225.5574	2031.6	1.173112	1222.752

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #1) ;

Substrate : N-nitrosodimethylamine
Culture : Lake Cochituate water
Condition : room temperature & pH 6-7

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
15	0
13.2	96
12.9	144
12.9	192
12.8	276
12.8	360
12.8	456
12.8	540
12.8	708
12.7	792
12.7	948
12.7	1116
12.7	1368
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.003647	---	15	123131.2	1.838812
(2-parameter)	0.002811	---	14.49780	120566.4	0.953238
First-order					
(1-parameter)	0.000262	---	15	121782.3	1.328333
(2-parameter)	0.000199	---	14.44349	118880.6	0.758977
Monod Kinetics					
(2-parameter)	-0.00003	-14.0093	15	54501.66	0.308885
(3-parameter)	-0.00003	-14.0058	14.9927	54487.99	0.308884

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #2) ;

Substrate : N-nitrosodimethylamine
Culture : Lake Cochituate water
Condition : room temperature & pH 6-7

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
1.5	0
1.37	96
1.31	144
1.28	192
1.25	276
1.22	360
1.2	456
1.19	540
1.18	708
1.18	792
1.18	948
1.17	1116
1.17	1368
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.000441	---	1.5	78953.97	0.015394
(2-parameter)	0.000301	---	1.408627	67837.68	0.006183
First-order					
(1-parameter)	0.000326	---	1.5	74694.94	0.011263
(2-parameter)	0.000225	---	1.403080	63472.53	0.004700
Monod Kinetics					
(2-parameter)	-0.00002	-1.41085	1.5	32425.17	0.000818
(3-parameter)	-0.00001	-1.39829	1.473	31904.24	0.000861

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #3) ;

Substrate : N-nitrosodimethylamine
Culture : Lake Cochituate water
Condition : room temperature & pH 6-7

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
0.15	0
0.136	96
0.131	144
0.128	192
0.119	276
0.111	360
0.109	456
0.107	540
0.105	708
0.104	792
0.104	948
0.103	1116
0.101	1368
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.000058	---	0.15	57869.93	0.000200
(2-parameter)	0.000043	---	0.139461	48439.72	0.000092
First-order					
(1-parameter)	0.000459	---	0.15	51361.43	0.000123
(2-parameter)	0.000350	---	0.138961	42950.83	0.000061
Monod Kinetics					
(2-parameter)	-0.00000	-0.14116	0.15	29132.39	0.000022
(3-parameter)	-0.00000	-0.13657	ERR	21725.37	ERR

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Kaplan,D.L. and Kaplan A.M. (data set #4) ;

Substrate : N-nitrosodimethylamine
Culture : Lake Cochituate water
Condition : room temperature & pH 6-7

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
0.015	0
0.0134	96
0.0129	144
0.0122	192
0.0111	276
0.0087	360
0.0069	456
0.0059	540
0.0056	708
0.0053	792
0.0051	948
0.005	1116
0.0049	1368
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.000011	---	0.015	37856.23	4.89E-06
(2-parameter)	0.000010	---	0.014025	35565.54	3.59E-06
First-order					
(1-parameter)	0.001169	---	0.015	26953.21	1.16E-06
(2-parameter)	0.001117	---	0.014399	26557.87	1.12E-06
Monod Kinetics					
(2-parameter)	-8.5E-06	-0.01686	0.015	21741.60	1.30E-06
(3-parameter)	-4.9E-06	-0.01303	ERR	19323.44	ERR

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Klecka,G.M.,et al (data set #1) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 8

Raw Data

S(ppb)	t(hr)
1600	0
1570	3
1470	14
1460	19
1420	27
530	50
110	55
10	70
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k*	K**	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	23.27621	---	1600	89.23920	48348.19
(2-parameter)	27.72168	---	1845.970	45.89039	35266.40
First-order					
(1-parameter)	0.060600	---	1600	301.7140	377353.4
(2-parameter)	0.081280	---	5706.572	132.2652	3284378.
Monod Kinetics					
(2-parameter)	21.59289	-32.4556	1600	87.94862	ERR
(3-parameter)	29.23791	22.50768	1861.978	45.57391	36058.56

* k has units of ppb/hr for zero-order/Monod kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #1) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 8

Raw Data

S (ppb)	t(hr)
1600	0
1570	3
1470	14
1460	19
1420	27
530	50
110	55
10	70
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 20.8 ppb
Yc = 0.136

Summary of results:

Kinetic Model	ko*	K**	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.284639	---	20.45139	59251.25
First-order (1-parameter)	0.000389	---	103.7004	81892.52
Monod Kinetics (2-parameter)	0.342334	159.7059	16.52735	9984.835

*ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb-hr for 1st-order kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Klecka,G.M.,et al (data set #2) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 9

Raw Data

S(ppb)	t(hr)
800	0
770	2
790	9
730	13
710	15
700	19
550	27
410	31
10	50
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k *	K**	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	13.77015	---	800	53.36714	10119.32
(2-parameter)	17.24581	---	925.8672	20.63294	6136.612
First-order					
(1-parameter)	0.077573	---	800	192.7163	127735.4
(2-parameter)	0.108348	---	3091.231	66.61709	965473.0
Monod Kinetics					
(2-parameter)	8.897153	-79.3392	800	29.79181	10523.60
(3-parameter)	11.99347	-59.1626	872.473	15.17606	5790.434

* k has units of ppb/hr for zero-order/Monod kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #2) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 9

Raw Data

S(ppb)	t(hr)
800	0
770	2
790	9
730	13
710	15
700	19
550	27
410	31
10	50
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko*	K**	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.369319	---	10.78251	2925.519
First-order (1-parameter)	0.000945	---	65.30591	23907.72
Monod Kinetics (2-parameter)	0.420010	60.59482	9.573569	830.2494

Bo = 11 ppb
Yc = 0.136

* ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb-hr for 1st-order kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Klecka,G.M.,et al (data set #3) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 9

Raw Data

S (ppb)	t(hr)
410	0
390	2
330	8
300	13
260	14
220	19
170	24
80	28
10	32
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k*	K**	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	11.34194	---	410	4.160506	535.2061
(2-parameter)	12.29912	---	432.4308	2.947864	445.9191
First-order					
(1-parameter)	0.085683	---	410	81.02445	10953.29
(2-parameter)	0.127002	---	1231.004	34.88447	115547.5
Monod Kinetics					
(2-parameter)	9.387858	-28.1195	410	1.357258	373.0343
(3-parameter)	9.810835	-26.0584	417.032	1.230424	310.6863

* k has units of ppb/hr for zero-order/Monod kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #3) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 9

Raw Data

S(ppb)	t(hr)
410	0
390	2
330	8
300	13
260	14
220	19
170	24
80	28
10	32
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko*	K**	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.324746	---	1.875002	348.4533
First-order (1-parameter)	0.001620	---	32.12857	3728.398
Monod Kinetics (2-parameter)	0.364380	27.12973	1.359894	229.7172

Bo = 18.9 ppb
Yc = 0.136

* ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb/hr for 1st-order kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Klecka,G.M.,et al (data set #4) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 8

Raw Data

S(ppb)	t(hr)
160	0
150	1
140	9
110	12
80	13
90	15
20	19
10	28
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k*	K**	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.790554	---	160	10.36879	347.6710
(2-parameter)	6.579330	---	174.7743	8.348174	361.3723
First-order					
(1-parameter)	0.092391	---	160	30.47460	1476.580
(2-parameter)	0.124351	---	313.0210	13.91000	5565.808
Monod Kinetics					
(2-parameter)	4.934976	-10.1036	160	9.884875	ERR
(3-parameter)	6.758245	1.576952	175.4876	8.343651	331.2070

* k has units of ppb/hr for zero-order/Monod kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Klecka,G.M.,et al (data set #4) ;

Substrate : pentachlorophenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 8

Raw Data

S (ppb)	t(hr)
160	0
150	1
140	9
110	12
80	13
90	15
20	19
10	28
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 19.3 ppb
Yc = 0.136

Summary of results:

Kinetic Model	ko*	K**	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.215716	---	7.845138	379.4158
First-order (1-parameter)	0.002896	---	20.42922	946.3390
Monod Kinetics (2-parameter)	0.227597	4.375302	7.804136	268.9583

* ko has units of ppb/ppb-hr for zero-order/Monod & 1/ppb-hr for 1st-order kinetics.
**K has units of ppb.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Larson,R.J.,Games,L.M.,et al (data set #1) ;

Substrate : octadecyltriammonium chloride
Culture : activated sludge
Condition : room temperature/neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
20	0
13	1.5
9	3
8	6
6	12
2	24
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.165618	---	20	25.56879	34.73946
(2-parameter)	0.822695	---	16.04255	20.20474	13.67511
First-order					
(1-parameter)	0.107531	---	20	6.593675	8.824162
(2-parameter)	0.089701	---	15.62538	3.813140	4.992541
Monod Kinetics					
(2-parameter)	-1.35472	-22.2365	20	1.836383	1.157857
(3-parameter)	-1.48572	-23.9068	17.5527	1.797975	2.006476

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Liu,D.,et al (data set #1) ; Substrate : Fenitrothrion
Culture : activated sludge
Condition : 22C & pH 6.8

um.pts.= 7

Raw Data

S(ppm)	t(hr)
9.9	0
9.57	21
9.66	45
9.53	51.5
9.53	69
9.53	93.5
9.29	165
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.004805	---	9.9	676.0062	0.015608
(2-parameter)	0.003850	---	9.817624	579.5018	0.008590
First-order					
(1-parameter)	0.000495	---	9.9	656.3725	0.014629
(2-parameter)	0.000399	---	9.817397	562.1416	0.008217
Monod Kinetics					
(2-parameter)	-0.00013	-9.95054	9.9	320.8411	0.004449
(3-parameter)	-0.00013	-9.94000	ERR	320.5061	ERR

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Liu,D.,et al (data set #2) ; Substrate : Fenitrothrion (w/co-metabolites)
Culture : activated sludge
Condition : 22C & pH 6.8

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
9.8	0
7.3	21
6.65	45
6.41	51.5
6	69
5.64	93.5
3.87	165
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.047324	---	9.8	516.8302	**1.157489**
(2-parameter)	0.035992	---	8.812374	361.8789	**0.468797**
First-order					
(1-parameter)	0.006424	---	9.8	227.3244	**0.406818**
(2-parameter)	0.005331	---	8.858890	134.6048	**0.228363**
Monod Kinetics					
(2-parameter)	-0.02959	-11.7614	9.8	54.14007	**0.079997**
(3-parameter)	-0.03263	-12.4386	9.3911	52.07240	**0.090172**

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Liu,D.,et al (data set #3) ; Substrate : 2,4-dichlorophenoxyacetic acid
Culture : activated sludge
Condition : 22C & pH 6.8

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9.9	0
9.7959	24
9.8958	72
7.4737	167
6.3441	191
2.5	240
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.025601	---	9.9	2649.192	1.736414
(2-parameter)	0.032983	---	11.46668	1326.636	1.443267
First-order					
(1-parameter)	0.004694	---	9.9	4866.443	3.913460
(2-parameter)	0.006542	---	14.83617	2354.164	7.341411
Monod Kinetics					
(2-parameter)	0.009073	-3.80103	9.9	990.4667	1.707499
(3-parameter)	0.011390	-3.65426	10.4559	508.0426	1.231720

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Lyons,C.D.,et al (data set #1) ;

Substrate : aniline
Culture : pond water
Condition : room temperature/neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
250	0
231	24
203	48
180	72
165	94
146	120
133	144
114	168
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.849494	---	250	38.62103	27.87055
(2-parameter)	0.816765	---	246.1540	32.49722	21.67907
First-order					
(1-parameter)	0.004515	---	250	12.97205	8.278910
(2-parameter)	0.004648	---	254.0636	9.142553	6.129229
Monod Kinetics					
(2-parameter)	2.996598	476.2840	250	8.245095	5.737687
(3-parameter)	4.173691	723.9386	251.84	7.692783	5.322062

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Lyons,C.D.,et al (data set #2) ;

Substrate : aniline
Culture : pond water (w/activated sludge)
Condition : room temperature/neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
250	0
81	24
47	48
32	72
19	96
13	120
11	144
10	168
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.205679	---	250	1304.471	6346.280
(2-parameter)	1.796770	---	208.8037	1233.287	3981.525
First-order					
(1-parameter)	0.023695	---	250	331.0626	628.9022
(2-parameter)	0.019883	---	164.0943	240.9366	1022.515
Monod Kinetics					
(2-parameter)	-2.49014	-191.708	250	58.82744	11.37712
(3-parameter)	-2.43998	-188.452	236.78	58.63813	32.99903

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Papanastasiou,A.C.,et al (data set #1) ;

Substrate : 2,4-dichlorophenoxyacetate
Culture : activated sludge
Condition : 20C & neutral pH

Num.pts.= 10

Raw Data

S(ppm)	t(hr)
96	0
95	20
94	38
86	64
73	88
72	92
65	98
60	103
40	115
15	120
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.472268	---	96	1096.443	244.5476
(2-parameter)	0.738237	---	124.0818	415.5604	226.4779
First-order					
(1-parameter)	0.010146	---	96	2379.698	653.5480
(2-parameter)	0.019187	---	257.4675	761.4244	3649.284
Monod Kinetics					
(2-parameter)	0.195637	-31.7640	96	360.4122	213.1756
(3-parameter)	0.270189	-30.3574	105.4198	151.3207	168.6407

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Papanastasiou,A.C.,et al (data set #2) ;

Substrate : glucose
Culture : activated sludge
Condition : 20C & neutral pH

Num.pts.= 9

Raw Data

S(ppm)	t(hr)
84	0
86	13
84	25
81	32
68	34
55	40
29	43
8	46
3	49
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.419510	---	84	307.2612	619.1344
(2-parameter)	2.578409	---	136.1234	82.09078	545.7554
First-order					
(1-parameter)	0.052577	---	84	492.4814	1698.106
(2-parameter)	0.107862	---	1084.495	119.9982	115511.0
Monod Kinetics					
(2-parameter)	0.766787	-14.4842	84	252.2095	428.2328
(3-parameter)	1.507363	-12.1246	116.4909	73.02659	325.7585

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Papanastasiou,A.C.,et al (data set #3) ;

Substrate : 2,4-dichlorophenoxyacetate
Culture : activated sludge
Condition : 20C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
56	0
55	9
53	21
46	33
35	45
22	49
9	58
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.682348	---	56	141.4780	65.87214
(2-parameter)	0.916168	---	67.56804	60.30922	50.62147
First-order					
(1-parameter)	0.024771	---	56	300.4690	181.2797
(2-parameter)	0.037234	---	106.5548	118.7703	500.5671
Monod Kinetics					
(2-parameter)	0.315942	-16.2117	56	73.16550	55.52088
(3-parameter)	0.434279	-14.6313	61.4454	36.11920	33.71611

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Papanastasiou,A.C.,et al (data set #4) ;

Substrate : glucose
Culture : activated sludge
Condition : 20C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
46	0
45	19
44	33
35	46
20	54
3	56
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.602089	---	46	384.1889	139.2729
(2-parameter)	0.985033	---	66.31450	143.0810	138.8303
First-order					
(1-parameter)	0.038734	---	46	689.4574	408.8487
(2-parameter)	0.073815	---	310.1791	227.3157	11977.69
Monod Kinetics					
(2-parameter)	0.264012	-10.4706	46	226.8518	111.1125
(3-parameter)	0.408556	-9.97438	54.5111	92.24164	94.78498

gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Radhakrishnan,I.,et al (data set #1) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

m.pts.= 10

Raw Data

(ppm)	t(hr)
416	0
393	1
357	2
310	3
262	4
200	5
132	6
67	7
20	8
4	9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	46.64099	---	416	0.245884	534.8923
(2-parameter)	51.41300	---	447.4585	0.114899	303.7122
First-order					
(1-parameter)	0.392374	---	416	4.924355	13460.28
(2-parameter)	0.569849	---	1571.554	1.770865	163320.0
Monod Kinetics					
(2-parameter)	44.63761	-6.06976	416	0.235683	ERR
(3-parameter)	53.22250	4.024885	450.5269	0.112270	284.7610

egression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

ata source -- Radhakrishnan,I.,et al (data set #1) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

um.pts.= 10

Raw Data

S(ppm)	t(hr)
416	0
393	1
357	2
310	3
262	4
200	5
132	6
67	7
20	8
4	9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 143 ppm
Yc = 0.609

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.203006	---	0.112838	625.8657
First-order (1-parameter)	0.001243	---	2.619798	6575.016
Monod Kinetics (2-parameter)	0.235515	29.21649	0.037376	68.85533

gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Radhakrishnan,I.,et al (data set #2) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

m.pts.= 10

Raw Data

(ppm)	t(hr)
850	0
831	1
793	2
762	3
695	4
635	5
565	6
490	7
400	8
300	9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	53.61948	---	850	0.763814	2196.005
(2-parameter)	63.67806	---	918.6512	0.293570	1190.398
First-order					
(1-parameter)	0.092626	---	850	2.090576	5927.188
(2-parameter)	0.120372	---	1034.881	0.820587	5989.162
Monod Kinetics					
(2-parameter)	24.46750	-324.852	850	0.195591	ERR
(3-parameter)	30.39471	-289.183	877.9886	0.089597	ERR

egression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

ata source -- Radhakrishnan,I.,et al (data set #2) : Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

im.pts.= 10

Raw Data

S(ppm)	t(hr)
850	0
831	1
793	2
762	3
695	4
635	5
565	6
490	7
400	8
300	9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 143 ppm
Yc = 0.609

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.216258	---	0.070397	155.6915
First-order (1-parameter)	0.000334	---	0.494467	1394.451
Monod Kinetics (2-parameter)	0.170402	-138.761	0.050227	150.5313

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Radhakrishnan,I.,et al (data set #3) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 30C & pH 7.1-7.5

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
850	0
832	1
808	2
788	3
748	4
705	5
655	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	29.09532	---	850	0.278272	235.5683
(2-parameter)	33.30780	---	869.3519	0.144189	159.9653
First-order					
(1-parameter)	0.038094	---	850	0.399251	325.8683
(2-parameter)	0.044751	---	876.6990	0.200504	246.7283
Monod Kinetics					
(2-parameter)	5.128027	-632.464	850	0.022146	ERR
(3-parameter)	5.629072	-623.486	852.927	0.017965	40.86270

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Radhakrishnan,I.,et al (data set #3) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 30C & pH 7.1-7.5

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
850	0
832	1
808	2
782	3
748	4
715	5
655	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

So = 155 ppm
Yc = 0.548

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order				
(1-parameter)	0.149174	---	0.102209	99.17299
First-order				
(1-parameter)	0.000192	---	0.173861	156.2925
Monod Kinetics				
(2-parameter)	0.037683	-580.414	0.011373	20.46545

gression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Radhakrishnan,I.,et al (data set #4) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

n.pts.= 10

Raw Data

S(ppm)	t(hr)*
404	0
15.7	1.83
15.7	2.16
15.7	2.58
15.7	3.07
15.7	3.97
15.7	4.5
15.7	7.75
11.2	12.35
7	15.38
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	65.11641	---	404	18.67616	79189.70
(2-parameter)	62.19605	---	386.5186	18.66826	72215.36
First-order					
(1-parameter)	4.487648	---	404	7.582871	176.7144
(2-parameter)	0.324266	---	40.23264	6.071859	13257.17
Monod Kinetics					
(2-parameter)	-67.5043	-26.9020	404	4.518309	7.184395
(3-parameter)	-67.7265	-405.345	405.3451	4.518275	7.364518

EFERS TO RESIDENCE TIME (V/Q)

ression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

a source -- Radhakrishnan,I.,et al (data set #5) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

.pts.= 10

Raw Data

(ppm)	t(hr)*
800	0
31.4	1.83
31.4	2.16
31.4	2.58
31.4	3.07
31.4	3.97
31.4	4.5
31.4	7.75
22	12.35
13.5	15.38
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	128.8841	---	800	18.66155	309989.3
(2-parameter)	122.8688	---	763.9844	18.65296	281599.3
First-order					
(1-parameter)	4.496391	---	800	7.204958	678.2094
(2-parameter)	0.345339	---	82.93864	5.819280	51517.85
Monod Kinetics					
(2-parameter)	-150.121	-56.5835	800	4.528569	32.97439
(3-parameter)	-150.727	-56.5776	803.2767	4.528528	34.04328

EFERS TO RESIDENCE TIME (V/Q)

gression of CSTR Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Radhakrishnan,I.,et al (data set #6) ; Substrate : phenol
Culture : Bacillus cereus
Condition : 40C & pH 7.1-7.5

m.pts.= 10

Raw Data

e(ppm)	t(hr)*
200	0
7.8	1.83
7.8	2.16
7.8	2.58
7.8	3.07
7.8	3.97
7.8	4.5
7.8	7.75
5	12.35
3.3	15.38
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	32.22881	---	200	18.64259	19364.00
(2-parameter)	30.64864	---	190.5361	18.63305	17502.77
First-order					
(1-parameter)	4.580519	---	200	6.483061	40.20607
(2-parameter)	0.340591	---	20.10174	5.005720	3241.826
Monod Kinetics					
(2-parameter)	-37.8698	-13.8961	200	3.700469	1.813562
(3-parameter)	-37.9921	-13.8950	200.6555	3.700443	1.856339

EFERS TO RESIDENCE TIME (V/Q)

:gression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ta source -- Saeger,V.W.,et al (data set #1) ;

Substrate : butyl benzyl phthalate
Culture : activated sludge
Condition : room temperature/neutral pH

m.pts.= 8

Raw Data

(ppm)	t(hr)
168	0
130	1
48	2
31	3
17	4
5	5
6	6
1	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	32.50553	---	168	1.160472	1226.166
(2-parameter)	29.12577	---	152.6902	1.104187	936.6944
First-order					
(1-parameter)	0.657416	---	168	0.306097	243.0274
(2-parameter)	0.727924	---	242.0448	0.215765	720.6662
Monod Kinetics					
(2-parameter)	112.3946	125.4480	168	0.158122	87.96731
(3-parameter)	127.6014	144.4310	175.7586	0.155826	83.24189

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Saeger,V.W.,et al (data set #2) ;

Substrate : butylglycolyl butyl phthalate
Culture : activated sludge
Condition : room temperature/neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
147	0
125	1
104	2
81	3
40	5
17	6
6	7
1	8
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	20.18935	---	147	0.121341	49.46017
(2-parameter)	19.55612	---	143.3494	0.111008	42.45441
First-order					
(1-parameter)	0.497406	---	147	2.288119	862.3758
(2-parameter)	0.648457	---	399.5179	1.091772	3009.782
Monod Kinetics					
(2-parameter)	24.36511	9.515216	147	0.007830	2.417022
(3-parameter)	24.94893	10.16930	148.6073	0.008453	2.188801

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Sayler,G.S.,et al (data set #1) ;

Substrate : phenol
Culture : activated sludge
Condition : 22C & neutral pH

um.pts.= 4

Raw Data

S(ppm)	t(hr)
30	0
14	4
4	8
1	12
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.859677	---	30	1.798082	14.70427
(2-parameter)	2.643041	---	28.10824	1.649926	11.52583
First-order					
(1-parameter)	0.270227	---	30	0.507754	3.732834
(2-parameter)	0.290937	---	36.68116	0.311326	12.82550
Monod Kinetics					
(2-parameter)	8.090299	19.86923	30	0.013215	0.074849
(3-parameter)	8.310990	20.53272	30.239	0.012602	0.083191

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Sayler,G.S.,et al (data set #2) ;

Substrate : phenol
Culture : activated sludge
Condition : 22C & neutral pH

im.pts.= 5

Raw Data

S(ppm)	t(hr)
30	0
22	4
13	8
8	12
1	24
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.487588	---	30	8.345172	18.46719
(2-parameter)	1.312248	---	27.39759	7.119816	12.26030
First-order					
(1-parameter)	0.133851	---	30	2.481637	6.208347
(2-parameter)	0.147139	---	38.08677	1.135238	13.98845
Monod Kinetics					
(2-parameter)	4.073899	20.20180	30	0.070560	0.272602
(3-parameter)	4.334966	21.81748	30.4677	0.061668	0.253835

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Shamat,N.A.,et al (data set #1) ;

Substrate : 3,5-dichlorobenzoate
Culture : mlsa
Condition : 20C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
50	0
50	120
50	312
46	720
44	744
35	1440
25	1920
10	2400
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.014467	---	50	93674.07	19.60572
(2-parameter)	0.017157	---	55.16960	39627.73	11.66542
First-order					
(1-parameter)	0.000549	---	50	254397.3	70.22563
(2-parameter)	0.000703	---	68.46946	118530.3	91.21325
Monod Kinetics					
(2-parameter)	0.007145	-14.3638	50	35538.27	14.12192
(3-parameter)	0.008832	-12.9370	52.46803	13853.78	5.990936

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Shamat,N.A.,et al (data set #1) ;

Substrate : 3,5-dichlorobenzoate
Culture : mlss
Condition : 20C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
50	0
50	120
50	312
46	720
44	744
35	1440
25	1920
10	2400
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 0.5 ppm
Yc = 0.15

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.007469	---	20203.11	5.059842
First-order (1-parameter)	0.000199	---	28964.48	4.446498
Monod Kinetics (2-parameter)	0.011531	20.60467	16422.52	0.794232

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Tanner,R.D.,et al (data set #1) ;

Substrate : glucose
Culture : pseudomonas ovalis
Condition : room temperature/neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
51833	0
50802	1
49541	2
48280	3
46118	4
41434	5
30085	6
17907	7
7404	8
2395	9
1250	10
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4962.506	---	51833	2.661244	65537053
(2-parameter)	6517.919	---	64139.59	0.937864	39843539
First-order					
(1-parameter)	0.307299	---	51833	7.458280	3.5E-08
(2-parameter)	0.460764	---	,193909.9	2.314333	2.5E-09
Monod Kinetics					
(2-parameter)	3676.869	-4746.80	51833	2.280213	ERR
(3-parameter)	5776.205	-1864.47	62619	0.917280	ERR

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Tanner,R.D.,et al (data set #1) :

Substrate : glucose
Culture : pseudomonas ovalis
Condition : room temperature/neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
51833	0
50802	1
49541	2
48280	3
46118	4
41434	5
30085	6
17907	7
7404	8
2396	9
1250	10
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 0.108 optical units
Yc = 0.00005 optical unit/ppm

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order*				
(1-parameter)	7189.096	---	0.271208	85036688
First-order**				
(1-parameter)	0.228958	---	1.197690	41826308
Monod Kinetics*				
(2-parameter)	9402.081	10055.17	0.168476	6471768.

* ko = (ppm/hr-optical unit)
**ko = (1/hr-optical unit)

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Taylor,B.F.,et al (data set #1) ;

Substrate : o-phthalic acid
Culture : activated sludge
Condition : 30C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
830	0
797	24
764	48
664	96
564	144
505	576
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.853227	---	830	12832.36	9341.919
(2-parameter)	0.735050	---	796.1208	11947.03	6454.976
First-order					
(1-parameter)	0.001234	---	830	11048.14	5394.732
(2-parameter)	0.001086	---	794.1978	10315.36	4048.513
Monod Kinetics					
(2-parameter)	-0.11838	-773.869	830	5097.962	3912.683
(3-parameter)	-0.09481	-742.649	763.3069	4471.934	5214.490

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Taylor,B.F.,et al (data set #2) ;

Substrate : o-phthalic acid
Culture : activated sludge
Condition : 30C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
830	0
780	24
681	48
664	96
624	144
349	576
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.985033	---	830	4761.788	4620.321
(2-parameter)	0.807721	---	774.2095	2689.831	1754.885
First-order					
(1-parameter)	0.001615	---	830	1695.098	1953.147
(2-parameter)	0.001450	---	783.3469	870.1143	954.0491
Monod Kinetics					
(2-parameter)	-0.73087	-1041.94	830	220.1061	436.8925
(3-parameter)	-0.75332	-1058.75	824.163	218.9489	429.9732

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Taylor,B.F.,et al (data set #3) ;

Substrate : o-phthalic acid
Culture : activated sludge
Condition : 30C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
830	0
797	24
714	48
598	96
481	144
17	576
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.555512	---	830	2140.369	5178.878
(2-parameter)	1.425074	---	783.7443	1577.994	3204.650
First-order					
(1-parameter)	0.006593	---	830	1172.340	11674.49
(2-parameter)	0.007052	---	1032.522	465.9583	10653.93
Monod Kinetics					
(2-parameter)	3.555686	317.5647	830	22.88305	143.3616
(3-parameter)	3.945901	369.8943	844.9293	12.24988	89.05183

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Wong,P.T.S. and Kaiser,K.L.E. (data set #1) ; Substrate : 4-chlorobiphenyl
Culture : acclimated Lake Ontaric
Condition : room temperature/neutre

Num.pts.= 4

Raw Data

S(ppm)	t(hr)
500	0
410	63
277	131
225	232
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.352350	---	500	495.6326	906.4386
(2-parameter)	1.303846	---	491.8596	481.8995	819.2364
First-order					
(1-parameter)	0.003728	---	500	291.0990	328.1329
(2-parameter)	0.003731	---	500.2549	291.0918	328.0446
Monod Kinetics					
(2-parameter)	-1.86659	-860.500	500	247.5029	359.1988
(3-parameter)	-1.30288	-692.296	532.1694	228.1958	599.1485

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Wong,P.T.S. and Kaiser,K.L.E. (data set #2) ; Substrate : 2-chlorobiphenyl
Culture : acclimated Lake Ontario bacteria
Condition : room temperature/neutral pH

Num.pts.= 4

Raw Data

S(ppm)	t(hr)
500	0
325	63
190	131
46	232
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.120506	---	500	233.1300	1048.279
(2-parameter)	1.973520	---	475.4299	180.7820	704.1071
First-order					
(1-parameter)	0.009632	---	500	378.4691	1289.097
(2-parameter)	0.010625	---	601.9028	233.8221	3080.665
Monod Kinetics					
(2-parameter)	3.724055	172.5652	500	6.096612	31.39973
(3-parameter)	3.608605	163.3364	496.2701	5.579831	29.21378

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Wong,P.T.S. and Kaiser,K.L.E. (data set #3) ; Substrate : biphenyl
Culture : acclimated Lake Ontario bacteria
Condition : room temperature/neutral pH

im.pts.= 4

Raw Data

S(ppm)	t(hr)
500	0
230	63
51	131
6	232
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.722879	---	500	1253.609	9294.350
(2-parameter)	2.460222	---	458.7636	1171.964	7093.539
First-order					
(1-parameter)	0.018467	---	500	137.4310	1372.312
(2-parameter)	0.019715	---	628.7591	76.85238	4734.003
Monod Kinetics					
(2-parameter)	10.94831	458.0843	500	17.01073	117.7629
(3-parameter)	11.87603	501.2731	512.0132	15.92989	143.3252

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Wong,P.T.S.,Liu,D.,et al (data set #1); Substrate : nitrilotriacetic acid
Culture : mutant bacteria
Condition : 20C & pH 7.0

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9750	0
9700	8
9550	24
6250	48
4000	80
3200	104
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	67.14660	---	9750	97.48716	439537.1
(2-parameter)	74.52112	---	10353.92	63.75936	354081.1
First-order					
(1-parameter)	0.010684	---	9750	99.24230	795525.2
(2-parameter)	0.012105	---	10993.70	45.87685	572599.5
Monod Kinetics					
(2-parameter)	125.8584	5519.553	9750	91.58107	528423.9
(3-parameter)	2002.004	159300.5	10949.63	45.85045	546205.9

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Wong,P.T.S.,Liu,D.,et al (data set #1); Substrate : nitrilotriacetic acid
Culture : mutant bacteria
Condition : 20C & pH 7.0

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9750	0
9700	8
9550	24
6250	48
4000	80
3200	104
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 0.0012 ppm
Yc = 0.1

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	2.009205	---	602.5051	3.4E+13
First-order (1-parameter)	0.000213	---	527.4954	5566421.
Monod Kinetics (2-parameter)	-0.14259	-9961.54	20.79889	105179.1

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Yordy,J.R.,et al (data set #1) ;

Substrate : N-nitrosodiethanolamine
Culture : Canyon Lake bacteria
Condition : 22C & pH 7.8

Num.pts.= 20

Raw Data

S(ppm)	t(hr)
1	0
0.97	24
0.99	48
1.09	72
1.04	96
1.01	120
0.89	144
0.93	168
0.92	192
0.8	216
0.74	240
0.61	264
0.41	312
0.26	336
0.13	360
0.1	384
0.02	408
0.014	432
0.007	456
0.005	504
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.002141	---	1	7001.852	0.032102
(2-parameter)	0.002875	---	1.283511	2023.515	0.016733
First-order					
(1-parameter)	0.008966	---	1	18304.64	0.199257
(2-parameter)	0.013552	---	6.857918	5148.531	3.043739
Monod Kinetics					
(2-parameter)	0.001925	-0.02797	1	6869.270	ERR
(3-parameter)	0.003148	0.024228	1.3105	1988.552	0.017174

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Yordy,J.R.,et al (data set #2) ;

Substrate : N-nitrosodiethanolamine
Culture : North Lake bacteria
Condition : 22C & pH 7.8

Num.pts.= 17

Raw Data

S(ppm)	t(hr)
1	0
1	24
0.94	72
1.01	96
1	120
0.94	168
0.96	192
0.91	240
0.79	264
0.79	288
0.71	312
0.54	336
0.4	384
0.22	432
0.04	480
0.03	528
0.02	600
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.001655	---	1	11113.74	0.030466
(2-parameter)	0.002255	---	1.266651	3512.063	0.017874
First-order					
(1-parameter)	0.005763	---	1	27202.95	0.171877
(2-parameter)	0.008757	---	4.345570	7687.769	1.253297
Monod Kinetics					
(2-parameter)	0.001169	-0.09805	1	9411.287	ERR
(3-parameter)	0.001961	-0.03911	1.2301	3429.460	ERR

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Yordy,J.R.,et al (data set #3) ;

Substrate : N-nitrosodiethanolamine
Culture : Canyon Lake bacteria
Condition : 22C & pH 7.8

um.pts.= 14

Raw Data

S(ppm)	t(hr)
0.05	0
0.049	24
0.05	48
0.051	72
0.049	96
0.028	120
0.024	144
0.008	168
0.009	192
0.014	216
0.004	240
0.001	264
0.003	288
0.001	312
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.000183	---	0.05	1792.847	0.000060
(2-parameter)	0.000224	---	0.059400	1114.213	0.000056
First-order					
(1-parameter)	0.011285	---	0.05	3580.978	0.000210
(2-parameter)	0.015501	---	0.141225	1321.403	0.000819
Monod Kinetics					
(2-parameter)	0.000226	0.004076	0.05	1680.017	0.000060
(3-parameter)	0.000380	0.011162	0.0653	829.9531	0.000049

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Yordy,J.R.,et al (data set #4) ;

Substrate : N-nitrosodiethanolamine
Culture : Canyon Lake bacteria
Condition : 22C & pH 7.8

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
0.05	0
0.047	24
0.05	48
0.051	72
0.049	96
0.047	120
0.029	144
0.025	168
0.009	192
0.011	216
0.004	240
0.001	264
0.003	288
0.001	312
0.001	336
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.000169	---	0.05	2330.840	0.000067
(2-parameter)	0.000214	---	0.061213	1190.683	0.000054
First-order					
(1-parameter)	0.011330	---	0.05	4586.443	0.000286
(2-parameter)	0.015842	---	0.168864	1473.412	0.001375
Monod Kinetics					
(2-parameter)	0.000190	0.002018	0.05	2291.707	0.000068
(3-parameter)	0.000347	0.009202	0.0675	960.4635	0.000060

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Yordy,J.R.,et al (data set #5) ;

Substrate : N-nitrosodiethanolamine
Culture : Canyon Lake bacteria
Condition : 22C & pH 7.8

im.pts.= 25

Raw Data

S(ppm)	t(hr)
0.045	0
0.045	24
0.04	48
0.046	72
0.046	96
0.046	120
0.045	144
0.046	168
0.046	192
0.046	216
0.044	240
0.039	264
0.045	288
0.037	312
0.04	336
0.039	360
0.022	384
0.023	408
0.017	432
0.02	456
0.004	480
0.003	504
0.0001	528
0.0001	576
0.0001	624

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.000072	---	0.045	23845.07	0.000124
(2-parameter)	0.000109	---	0.063223	6768.866	0.000081
First-order					
(1-parameter)	0.008753	---	0.045	49546.44	0.000696
(2-parameter)	0.014691	---	1.086374	13478.09	0.081610
Monod Kinetics					
(2-parameter)	0.000058	-0.00206	0.045	22635.72	0.000078
(3-parameter)	0.000102	-0.00065	0.062	6730.221	ERR

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Yordy,J.R.,et al (data set #6) ;

Substrate : N-nitrosodiethanolamine
Culture : sewage
Condition : 22C & pH 7.8

ım.pts.= 25

Raw Data

S(ppm)	t(hr)
1	0
0.95	24
1	72
1.03	120
1	144
0.93	192
0.89	216
0.83	264
0.79	312
0.77	336
0.67	384
0.65	408
0.58	432
0.44	456
0.56	480
0.48	504
0.44	528
0.32	552
0.26	576
0.21	600
0.14	672
0.11	744
0.06	792
0.05	814
0.03	864

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.001147	---	1	7559.095	0.009953
(2-parameter)	0.001407	---	1.157833	2779.628	0.005504
First-order					
(1-parameter)	0.003046	---	1	36075.43	0.067779
(2-parameter)	0.004507	---	2.665134	9855.020	0.261582
Monod Kinetics					
(2-parameter)	0.001011	-0.05036	1	7105.522	ERR
(3-parameter)	0.001533	0.032263	1.176	2712.667	0.005628

Appendix E

Compilation of Regression Analysis Results for Aerobic Biodegradation Data from Previous NJIT MS Theses

Table of Contents

List of MS Theses

1. Colish, J., "Biodegradation of Phenol and o-Chlorophenol Using Activated Sludge Bacteria," MS Thesis, New Jersey Institute of Technology (1984).

2. Gonnaphula, P., "Biodegradation of Mixed Phenolic Substrates," New Jersey Institute of Technology (1986).

3. McMullen, N., "A Comparison of the Biodegradation of Phenol and o-Chlorophenol Using a Municipal Mixed Liquor and Three Commercial Microbial Populations," New Jersey Institute of Technology (1985).

4. Naik, N., "Biodegradation of Multiple Substrates in a Batch Reactor," New Jersey Institute of Technology (1986).

5. Pak, K., "Biodegradation of Phenolics Using Mixed Liquor from Passaic Valley Sewerage Commissioner's Plant (Newark, NJ)," New Jersey Institute of Technology (1985).

6. Salerno, S., "A Comparison of the Biodegradation of Nitrobenzene, 1-Butanol and 2,4-Dichlorophenoxyacetic Acid Using a Municipal Mixed Liquor and Three Commercial Microbial Populations," New Jersey Institute of Technology (1984).

Index of Batch Reactor Data Analysis Results

MS Thesis	Substrate	Medium	Biomass Type	# Sets	Page
4	Phenol	Activated sludge	Constant	6	E-58, E-61, E-64, E-67, E-70, E-73
	2-chlorophenol	Activated sludge	Constant	4	E-76, E-79, E-82, E-85
	Nitrobenzene	Activated sludge	Constant	12	E-59, E-62, E-65, E-68, E-71, E-74, E-77, E-80, E-83, E-86, E-88, E-90
	2,6-dichloro-phenol	Activated sludge	Constant	12	E-60, E-63, E-66, E-69, E-72, E-75, E-78, E-81, E-84, E-87, E-89, E-91
5	2,6-dichloro-phenol	Activated sludge	Constant	4	E-92, E-94, E-95, E-97
			Variable	2	E-93, E-96
	2-chlorophenol	Activated sludge	Constant	4	E-98, E-100, E-101, E-103
			Variable	2	E-99, E-102
	Phenol	Activated sludge	Constant	2	E-104, E-106
			Variable	1	E-105
6	2,4-dichloro-phenol	Activated sludge	Constant	1	E-107
			Variable	1	E-108

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #1)*;

Substrate : phenol
Culture : mlss
Condition : room temperature & pH 6.9

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
133.687	0
121.007	0.333
103.234	0.667
91.888	1
43.417	1.333
31.503	1.667
15.27	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	59.69328	---	133.687	0.023342	83.17603
(2-parameter)	65.98901	---	143.1327	0.015788	68.75395
First-order					
(1-parameter)	0.937721	---	133.687	0.099541	453.1816
(2-parameter)	1.191976	---	201.4727	0.042335	846.9925
Monod Kinetics					
(2-parameter)	50.52592	-10.2532	133.687	0.021424	ERR
(3-parameter)	65.70776	-0.25146	143.149	0.015788	68.80046

* corresponds to data extracted from Table 20 on page 92.

egression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

ta source -- Colish Thesis (data set #1)*;

Substrate : phenol
Culture : mlss
Condition : room temperature & pH 6.9

n.pts.= 7

Raw Data	
(ppm)	t(hr)
33.687	0
21.007	0.333
03.234	0.667
91.888	1
43.417	1.333
31.503	1.667
15.27	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order				
(1-parameter)	0.061106	---	0.016304	64.89691
First-order				
(1-parameter)	0.000892	---	0.072210	319.4442
Monod Kinetics				
(2-parameter)	0.058391	-3.16082	0.016189	73.95568

Bo = 811 ppm**
Yc = 3.51**

* corresponds to data extracted from Table 20 on page 92.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #2)* ;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
19.584	0
17.922	1
18.192	2
13.758	3
11.853	4
7.523	5
6.042	6
2.319	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.300781	---	19.584	0.372121	1.969858
(2-parameter)	2.643967	---	21.40301	0.187367	1.309804
First-order					
(1-parameter)	0.240721	---	19.584	1.880993	10.89052
(2-parameter)	0.323747	---	31.41657	0.777067	23.14026
Monod Kinetics					
(2-parameter)	1.742893	-2.49510	19.584	0.272139	ERR
(3-parameter)	2.197223	-1.53308	20.9563	0.168417	1.033465

* corresponds to data extracted from Table 21 on page 93.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #2)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
19.584	0
17.922	1
18.192	2
13.758	3
11.853	4
7.523	5
6.042	6
2.319	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 1780 ppm**
Yc = 4.05**

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.001272	---	0.359394	1.887232
First-order (1-parameter)	0.000132	---	1.829427	10.55572
Monod Kinetics (2-parameter)	0.000972	-2.43761	0.267972	ERR

* corresponds to data extracted from Table 21 on page 93.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #3) *;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0-7.5

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
19.121	0
15.922	1
10.561	2
4.582	3
0.915	4
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.579907	---	19.121	0.027827	0.583687
(2-parameter)	4.821304	---	19.86280	0.019125	0.444572
First-order					
(1-parameter)	0.654863	---	19.121	0.559246	13.77335
(2-parameter)	0.841562	---	36.05035	0.259236	60.93097
Monod Kinetics					
(2-parameter)	4.469234	-0.18508	19.121	0.027487	0.579291
(3-parameter)	5.030178	0.284219	19.9701	0.018605	0.444091

* corresponds to data extracted from Table 22 on page 94.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #3) *;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0-7.5

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
19.121	0
15.922	1
10.561	2
4.582	3
0.915	4
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 1540 ppm **
Yc = 7.57 **

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.002865	---	0.024874	0.519680
First-order (1-parameter)	0.000400	---	0.525563	12.88930
Monod Kinetics (2-parameter)	0.002857	-0.01946	0.024871	0.520128

* corresponds to data extracted from Table 22 on page 94.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #4)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 6.9-7.0

Num.pts.= 4

Raw Data

S(ppm)	t(hr)
19.81	0
17.409	1
9.754	2
4.049	3
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.090507	---	19.81	0.072247	1.872166
(2-parameter)	5.687617	---	21.28692	0.042596	1.377952
First-order					
(1-parameter)	0.481747	---	19.81	0.225790	7.989178
(2-parameter)	0.587313	---	26.07041	0.112945	12.69590
Monod Kinetics					
(2-parameter)	3.584341	-3.23868	19.81	0.057111	ERR
(3-parameter)	4.545312	-2.04432	20.9257	0.039514	1.074630

* corresponds to data extracted from Table 23 on page 95.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #4)* ;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 6.9-7.0

Num.pts.= 4

Raw Data

S(ppm)	t(hr)
19.81	0
17.409	1
9.754	2
4.049	3
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 1350 ppm **
Yc = 4.44 **

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.003685	---	0.069411	1.764423
First-order (1-parameter)	0.000346	---	0.217821	7.666642
Monod Kinetics (2-parameter)	0.002638	-3.13219	0.056018	ERR

* corresponds to data extracted from Table 23 on page 95.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #5)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.3-7.8

Num.pts.= 14

Raw Data

S(ppm)	t(hr)
36.927	0
37.568	0.5
38.144	1
36.131	1.5
33.3	2
30.978	2.5
28.965	3
23.106	4
20.916	4.5
14.635	5
11.547	5.5
7.678	6
2.461	6.5
0.385	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.707972	---	36.927	0.873985	19.37188
(2-parameter)	5.973828	---	43.96132	0.222733	7.948607
First-order					
(1-parameter)	0.441735	---	36.927	4.994257	167.7205
(2-parameter)	0.695776	---	173.1284	1.696725	2094.281
Monod Kinetics					
(2-parameter)	3.814060	-2.57171	36.927	0.686266	15.46543
(3-parameter)	5.137828	-1.65120	42.7478	0.184048	ERR

* corresponds to data extracted from Table 24 on page 96.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #5)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 6.9-7.0

Num.pts.= 14

Raw Data

S(ppm)	t(hr)
36.927	0
37.568	0.5
38.144	1
36.131	1.5
33.3	2
30.978	2.5
28.965	3
23.106	4
20.916	4.5
14.635	5
11.547	5.5
7.678	6
2.461	6.5
0.385	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 780 ppm **
Yc = 2.38 **

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.005770	---	0.816730	17.66430
First-order (1-parameter)	0.000521	---	4.780547	158.1892
Monod Kinetics (2-parameter)	0.004724	-2.52899	0.653413	14.34113

* corresponds to data extracted from Table 24 on page 96.
** estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #6)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0-7.3

Num.pts.= 20

Raw Data

S(ppm)	t(hr)
39.764	0
43.189	0.5
37.345	1
37.795	1.5
37.84	2
36.375	2.5
35.582	3.5
34.108	4
32.016	4.5
28.447	5
27.311	5.5
24.139	6
21.793	6.5
19.779	7
17.066	7.5
14.474	8
11.968	8.5
10.338	9
7.365	9.5
0.75	10.5
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.137690	---	39.764	1.601205	15.76403
(2-parameter)	3.969826	---	46.21755	0.467145	7.361992
First-order					
(1-parameter)	0.222962	---	39.764	10.73131	131.1092
(2-parameter)	0.365603	---	133.7009	3.566880	987.7162
Monod Kinetics					
(2-parameter)	2.536906	-3.47718	39.764	1.172813	12.13608
(3-parameter)	3.356384	-2.37681	44.937	0.365404	5.366433

* corresponds to data extracted from Table 25 on page 97.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #6)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0-7.3

Num.pts.= 20

Raw Data

S(ppm)	t(hr)
39.764	0
43.189	0.5
37.345	1
37.795	1.5
37.84	2
36.375	2.5
35.582	3.5
34.108	4
32.016	4.5
28.447	5
27.311	5.5
24.139	6
21.793	6.5
19.779	7
17.066	7.5
14.474	8
11.968	8.5
10.338	9
7.365	9.5
0.75	10.5
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 730 ppm **
Yc = 2.74 **

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order				
(1-parameter)	0.004078	---	1.447083	14.01920
First-order				
(1-parameter)	0.000275	---	9.981147	118.8475
Monod Kinetics				
(2-parameter)	0.003339	-3.39594	1.094488	10.91781

* corresponds to data extracted from Table 25 on page 97.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Colish Thesis (data set #7)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0-7.3

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
39.665	0
36.011	0.5
37.724	1
37.165	1.5
39.422	2
34.92	2.5
29.626	3
27.539	3.5
23.711	4
19.209	4.5
13.895	5
11.804	5.5
8.317	6
4.337	6.5
1.146	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.027012	---	39.665	0.767499	19.39536
(2-parameter)	6.276865	---	46.26842	0.301037	11.86059
First-order					
(1-parameter)	0.343322	---	39.665	3.619149	124.5127
(2-parameter)	0.523687	---	112.7548	1.216559	624.1664
Monod Kinetics					
(2-parameter)	4.033279	-3.39825	39.665	0.635152	ERR
(3-parameter)	5.595220	-1.60620	45.3653	0.287857	ERR

E1-8

* corresponds to data extracted from Table 26 on page 98.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Colish Thesis (data set #7)*;

Subatrate : o-chlorophenol
Culture : mlss
Condition : room temperature & pH 7.0-7.3

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
39.665	0
36.011	0.5
37.724	1
37.165	1.5
39.422	2
34.92	2.5
29.626	3
27.539	3.5
23.711	4
19.209	4.5
13.895	5
11.804	5.5
8.317	6
4.337	6.5
1.146	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 790 ppm **
Yc = 1.95 **

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.006128	---	0.727958	17.92901
First-order (1-parameter)	0.000407	---	3.455815	117.6294
Monod Kinetics (2-parameter)	0.004972	-3.30753	0.613613	ERR

* corresponds to data extracted from Table 26 on page 98.
** estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #1A)*;

Substrate : phenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
108.49	0
108.9	2
80	3.83
35.47	22.67
23.85	24.67
11.25	26.67
4	28.67
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.567632	---	108.49	4.030620	51.30173
(2-parameter)	3.562052	---	108.3540	4.030091	51.13468
First-order					
(1-parameter)	0.089824	---	108.49	33.86366	137.3189
(2-parameter)	0.107187	---	169.6750	25.59248	880.9398
Monod Kinetics					
(2-parameter)	3.418923	-1.79127	108.49	3.974623	49.23132
(3-parameter)	3.383009	-1.96308	107.9545	3.966439	48.37053

* simultaneous biodegradation with data set #1B extracted from Table 1 on page 21 of Mr.Prasad Gonnaphula thesis.

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Prasad Thesis (data set #1B) *;

Substrate : 2,6-dichlorophenol
Culture : mlss
Condition : 25C & neutral pH

im.pts.= 12

Raw Data

S(ppm)	t(hr)
10.47	0
10.19	2
10.98	3.83
7.09	22.67
6.92	24.67
5.8	26.67
5.6	28.67
4	46.42
3.8	52.67
2	69.92
1.14	93.92
1.07	97.67
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.116411	---	10.47	90.46166	1.225898
(2-parameter)	0.108999	---	10.01605	84.58750	1.004968
First-order					
(1-parameter)	0.022768	---	10.47	18.36263	0.347274
(2-parameter)	0.024312	---	11.64468	9.533379	0.272336
Monod Kinetics					
(2-parameter)	0.452896	14.99458	10.47	9.179072	0.187843
(3-parameter)	0.712344	25.20597	11.0246	7.264935	0.152661

* simultaneous biodegradation with data set #1A from Table 1 on page 21 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #2A)*;

Substrate : phenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
125.5	0
111.26	2
93.62	3.83
38.36	22.66
25.49	24.66
10	26.66
2	28.66
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.228931	---	125.5	3.083651	55.14758
(2-parameter)	3.993908	---	119.9213	2.443923	38.98375
First-order					
(1-parameter)	0.108746	---	125.5	48.62556	185.4662
(2-parameter)	0.135781	---	251.5209	35.61662	3784.648
Monod Kinetics					
(2-parameter)	4.089217	-1.45406	125.5	3.027567	53.07956
(3-parameter)	3.669773	-3.06352	119.0558	2.167546	ERR

* simultaneous biodegradation with data set #2B extracted from Table 2 on page 22 of Mr. Prasad Gonnaphula' thesis.

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Prasad Thesis (data set #2B) *;

Substrate : 2,6-dichlorophenol
Culture : mlss
Condition : 25C & neutral pH

um.pts.= 11

Raw Data

S(ppm)	t(hr)
11.25	0
10.98	2
11.09	3.83
7.7	22.66
7.6	24.66
7.6	26.66
7.5	28.66
5.6	46.41
4.7	70.41
2.2	97.41
1.48	100.66
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.103072	---	11.25	58.25085	0.618851
(2-parameter)	0.094600	---	10.70453	45.97790	0.411464
First-order					
(1-parameter)	0.017374	---	11.25	70.58592	0.330539
(2-parameter)	0.018747	---	12.43179	56.16196	0.469982
Monod Kinetics					
(2-parameter)	0.187596	5.013734	11.25	27.91734	0.228173
(3-parameter)	0.167683	4.081023	11.0526	27.20457	0.224083

* simultaneous biodegradation with data set #2A extracted from Table 2 on page 22 of Mr.Prasad Gonnaphula's thesis.

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Prasad Thesis (data set #3A)*;

Substrate : phenol
Culture : mlss
Condition : 25C & neutral pH

um.pts.= 8

Raw Data

S(ppm)	t(hr)
141.67	0
124.7	2
89.8	4.5
80	6.5
30.99	21
10	24
2	26
1	28
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.513798	---	141.67	6.837301	207.8674
(2-parameter)	4.877881	---	128.3103	4.623498	110.0102
First-order					
(1-parameter)	0.149776	---	141.67	24.97919	257.2702
(2-parameter)	0.177326	---	275.5087	17.98153	3058.028
Monod Kinetics					
(2-parameter)	7.393144	13.79008	141.67	4.075077	133.4083
(3-parameter)	6.184920	8.760533	131.3525	3.304372	91.69711

* simultaneous biodegradation with data set #3B extracted from Table 3 on page 23 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #3B) *;

Substrate : 2,6-dichlorophenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
11.9	0
11.5	2
11	4.5
11	6.5
8.6	21
8.5	24
8.4	26
8.42	28
4.32	45.75
1.87	69.75
1.31	73
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.146945	---	11.9	6.063998	0.130939
(2-parameter)	0.147265	---	11.91573	6.058904	0.131399
First-order					
(1-parameter)	0.026391	---	11.9	69.98139	2.100899
(2-parameter)	0.030542	---	15.01913	35.50347	2.915359
Monod Kinetics					
(2-parameter)	0.153414	0.257977	11.9	5.933052	0.128136
(3-parameter)	0.160144	0.445837	11.9958	5.817634	0.129501

* simultaneous biodegradation with data set #3A extracted from Table 3 on page 23 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #4A)*;

Substrate : phenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
117.35	0
120.65	1
118	3
60.5	20.5
19.7	22.66
9.7	23.66
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.116148	---	117.35	10.88367	184.3986
(2-parameter)	4.615138	---	128.7906	7.540630	160.6116
First-order					
(1-parameter)	0.087106	---	117.35	34.45190	440.0987
(2-parameter)	0.105856	---	180.6964	24.60526	1262.869
Monod Kinetics					
(2-parameter)	2.255019	-22.9347	117.35	4.527771	260.9559
(3-parameter)	2.478862	-22.7904	123.3504	2.492133	240.1667

* simultaneous biodegradation with data set #4B extracted from Table 4 on page 24 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #4B)*;

Substrate : 2,6-dichlorophenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 4

Raw Data

S(ppm)	t(hr)
10.55	0
10.75	1
10.25	3
1.85	20.5
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.423457	---	10.55	1.855224	0.332671
(2-parameter)	0.451138	---	11.11322	0.694579	0.141364
First-order					
(1-parameter)	0.084796	---	10.55	2.141862	1.350539
(2-parameter)	0.090505	---	11.85466	0.901786	0.795613
Monod Kinetics					
(2-parameter)	0.124772	-3.52800	10.55	1.571155	4.366994
(3-parameter)	0.154366	-3.28496	10.815	0.536337	3.036660

* simultaneous biodegradation with data set #4A extracted from Table 4 on page 24 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #5A)*;

Substrate : phenol
Culture : mlss
Condition : 21C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
101.5	0
107.8	1
101.6	2.5
95.4	5
93.2	6.75
21.67	23.75
8.25	25.08
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.526172	---	101.5	6.753561	83.97305
(2-parameter)	3.963098	---	111.9107	1.977485	31.05867
First-order					
(1-parameter)	0.086600	---	101.5	15.86222	416.2422
(2-parameter)	0.099927	---	140.2438	8.340169	369.7765
Monod Kinetics					
(2-parameter)	2.422181	-13.2765	101.5	5.732733	58.55281
(3-parameter)	2.853630	-11.7127	109.579	1.413480	19.01571

* simultaneous biodegradation with data set #5B extracted from Table 5 of page 25 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #5B)*;

Substrate : 2,6-dichlorophenol
Culture : mlss
Condition : 21C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
11.5	0
11.9	1
11.3	2.5
10.7	5
9.95	6.75
2.1	23.75
1.2	25.08
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.398463	---	11.5	3.679809	0.584256
(2-parameter)	0.437293	---	12.38167	1.017124	0.194500
First-order					
(1-parameter)	0.081561	---	11.5	9.180131	3.712160
(2-parameter)	0.092062	---	14.74245	4.143625	2.773285
Monod Kinetics					
(2-parameter)	0.244136	-1.93540	11.5	2.693235	ERR
(3-parameter)	0.312788	-1.38735	12.1419	0.735803	ERR

* simultaneous biodegradation with data set #5A extracted from Table 5 on page 25 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #6A)*;

Substrate : phenol
Culture : mlss
Condition : 21C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
140.6	0
142.5	0.42
128.5	1.42
114.5	2.42
112.5	3.42
100	4.42
85.5	6.42
64	9.42
41	11.42
9.7	23.58
5.4	25.58
1.2	27.91
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	5.916785	---	140.6	7.602918	266.1656
(2-parameter)	5.353486	---	130.7255	6.228442	178.5060
First-order					
(1-parameter)	0.140308	---	140.6	8.443000	285.0632
(2-parameter)	0.155950	---	197.8322	5.481822	588.2982
Monod Kinetics					
(2-parameter)	11.08087	39.69368	140.6	1.326783	23.83599
(3-parameter)	10.61288	37.12099	138.7603	1.310690	22.06392

* simultaneous biodegradation with data set #6B extracted from Table 6 on page 26 of Mr. Prasad Gonnanhula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #6B)*;

Substrate : 2-chlorophenol
Culture : mlss
Condition : 21C & neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
13.6	0
14.1	0.42
12.7	1.42
12.1	2.42
12	3.42
11.9	4.42
10.5	6.42
10.2	9.42
10	11.42
3	23.58
1.9	25.58
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.442663	---	13.6	1.738072	0.340576
(2-parameter)	0.457818	---	13.86600	1.548994	0.324665
First-order					
(1-parameter)	0.067775	---	13.6	9.507647	2.927212
(2-parameter)	0.077272	---	16.45877	5.341382	3.119672
Monod Kinetics					
(2-parameter)	0.346385	-1.49087	13.6	1.336737	ERR
(3-parameter)	0.353428	-1.41253	13.6389	1.333352	ERR

* simultaneous biodegradation with data set #6A extracted from Table 6 on page 26 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #7A)*;

Substrate : phenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
165	0
180	0.66
168.9	1.66
164.5	2.66
162.3	3.66
138	4.66
134.9	5.66
110.73	6.66
87.9	7.66
75.2	8.66
3.5	23.82
1.5	25.15
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	7.179689	---	165	5.447407	280.8026
(2-parameter)	7.756591	---	174.7984	4.492372	270.2822
First-order					
(1-parameter)	0.168835	---	165	9.617379	2283.095
(2-parameter)	0.197472	---	303.0373	2.488874	2720.823
Monod Kinetics					
(2-parameter)	11.06851	25.13694	165	3.329401	290.5795
(3-parameter)	18.49789	58.09850	194.9005	0.900779	143.9922

* simultaneous biodegradation with data set #7B extracted from Table 7 on page 27 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #7B)*;

Substrate : 2-chlorophenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
15.6	0
16.5	0.66
16.4	1.66
16.1	2.66
16	3.66
15.48	4.66
15.3	5.66
14.5	6.66
14	7.66
12.06	8.66
2.67	23.82
1.32	25.15
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.544637	---	15.6	11.89281	3.527769
(2-parameter)	0.644086	---	17.87365	2.039351	0.846019
First-order					
(1-parameter)	0.086525	---	15.6	17.69535	16.35073
(2-parameter)	0.103725	---	23.45146	5.096931	11.42300
Monod Kinetics					
(2-parameter)	0.366309	-2.14707	15.6	11.17434	ERR
(3-parameter)	0.508786	-1.36006	17.5209	1.893260	ERR

* simultaneous biodegradation with data set #7A extracted from Table 7 on page 27 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #8A)* ;

Substrate : phenol
Culture : mlss
Condition : 25C & neutral pH]

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
95.5	0
94.5	1
93	2
83	3
74.6	4
64.9	5
52.61	7
37	8
13.88	9
4.28	10
2.8	11
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	8.176642	---	95.5	1.425481	95.30410
(2-parameter)	9.825702	---	109.6011	0.529260	51.09712
First-order					
(1-parameter)	0.266653	---	95.5	7.817324	807.2108
(2-parameter)	0.384366	---	288.0366	2.842221	4678.628
Monod Kinetics					
(2-parameter)	6.076627	-8.99048	95.5	0.924666	ERR
(3-parameter)	7.858893	-6.06117	105.4963	0.418316	ERR

* simultaneous biodegradation with data set #8B extracted from Table 8 on page 28 of Mr. Prasad Gonnaphula's thesis.

Regresaion of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #8B)*;

Substrate : 2-chlorophenol
Culture : mlss
Condition : 25C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
10.75	0
11.76	1
12.3	2
12.25	3
12	4
11.53	5
10.57	7
8.85	8
7.39	9
5.26	10
4.41	11
3.2	12
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.614137	---	10.75	17.99957	6.788812
(2-parameter)	0.915405	---	14.68159	3.145581	2.635894
First-order					
(1-parameter)	0.086067	---	10.75	17.28262	9.189680
(2-parameter)	0.130804	---	18.55404	3.836381	9.043135
Monod Kinetics					
(2-parameter)	-71.4453	-837.089	10.75	17.28257	9.214332
(3-parameter)	0.542382	-2.97377	13.9236	3.003903	ERR

* simultaneous biodegradation with data set #8A extracted from Table 8 on page 28 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #9A)*;

Substrate : phenol
Culture : mlss
Condition : 27C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
150	0
140.2	1
114.3	2
90.5	3
80.3	4
67.5	5
50.3	6
41	7
22	8
10.31	9
3.2	10
1.2	11
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	15.32631	---	150	0.309408	72.67871
(2-parameter)	14.58328	---	144.4422	0.272827	58.02283
First-order					
(1-parameter)	0.342623	---	150	4.395642	774.7662
(2-parameter)	0.466073	---	436.9515	1.782996	8833.824
Monod Kinetics					
(2-parameter)	18.73802	11.40344	150	0.054849	13.56828
(3-parameter)	19.06536	11.93332	151.1734	0.053951	13.62580

* simultaneous biodegradation with data set #9B extracted from Table 9 on page 29 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #9B)*;

Substrate : 2-chlorophenol
Culture : mlss
Condition : 27C & neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
21.93	0
22.15	1
19.58	2
17.3	3
14.7	4
11.6	5
8.9	6
7.3	7
5.1	8
2.1	9
1.1	10
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.097752	---	21.93	0.290129	1.276733
(2-parameter)	2.329542	---	23.62589	0.103790	0.563245
First-order					
(1-parameter)	0.236036	---	21.93	3.598483	17.17133
(2-parameter)	0.320723	---	43.22241	1.312364	52.96274
Monod Kinetics					
(2-parameter)	1.966904	-0.60901	21.93	0.276014	ERR
(3-parameter)	2.458725	0.462633	23.8062	0.099470	0.551961

* simultaneous biodegradation with data set #9A extracted from Table 9 on page 29 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #10A) *;

Substrate : phenol
Culture : mlss
Condition : 27C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
145	0
130	1
80	3
62.5	4
42.1	5
22.1	6
10.1	7
1.23	8
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	19.50845	---	145	0.098237	37.38724
(2-parameter)	19.21655	---	143.2991	0.096149	35.50555
First-order					
(1-parameter)	0.452495	---	145	3.028190	707.6333
(2-parameter)	0.629261	---	463.5631	1.350823	14569.98
Monod Kinetics					
(2-parameter)	22.48225	7.637038	145	0.014807	6.044217
(3-parameter)	23.29478	8.497656	147.6562	0.011461	4.628010

* simultaneous biodegradation with data set #10B extracted from Table 10 on page 30 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #10B)*;

Substrate : 2-chlorophenol
Culture : mlss
Condition : 27C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
21	0
20	1
16.7	3
12.3	4
9.7	5
5.6	6
2.7	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.440650	---	21	0.364570	2.171664
(2-parameter)	2.793189	---	22.94613	0.182808	1.426252
First-order					
(1-parameter)	0.237444	---	21	1.964511	11.85994
(2-parameter)	0.318571	---	33.76646	0.874418	30.70920
Monod Kinetics					
(2-parameter)	1.715196	-3.26764	21	0.201337	ERR
(3-parameter)	2.054816	-2.57809	22.1695	0.126337	ERR

* simultaneous biodegradation with data set #10A extracted from Table 10 on page 30 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #11A)* ;

Substrate : phenol
Culture : mlss
Condition : 31C & neutral pH

Num.pts.= 14

Raw Data

S(ppm)	t(hr)
122.5	0
127.9	1
127.33	2
121.66	3
118.02	4
105.5	5
80.5	6.25
29.9	22.75
22.5	23.75
16.5	25
3.5	26.16
2.5	27.32
1.6	28.8
1	30.3
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.271858	---	122.5	3.845950	70.18389
(2-parameter)	4.563115	---	129.8467	2.686988	55.94853
First-order					
(1-parameter)	0.132265	---	122.5	33.86905	621.5093
(2-parameter)	0.161255	---	266.3904	21.05997	2748.237
Monod Kinetics					
(2-parameter)	4.495504	1.858292	122.5	3.754767	68.07259
(3-parameter)	5.055253	3.589436	131.1224	2.427145	50.25916

* simultaneous biodegradation with data set #11B extracted from Table 11 on page 31 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #11B)*;

Substrate : nitrobenzene
Culture : mlss
Condition : 31C & neutral pH

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
19	0
19	1
19.9	2
19.78	3
18.65	4
17.07	5
16.2	6.25
9.23	22.75
8.8	23.75
8.3	25
5.8	26.16
4	27.32
1.5	28.8
1.08	30.3
1.01	30.9
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.538576	---	19	10.07260	2.921702
(2-parameter)	0.607473	---	20.85490	5.707882	2.106347
First-order					
(1-parameter)	0.075982	---	19	61.21094	13.63091
(2-parameter)	0.099600	---	36.82137	35.88558	57.43534
Monod Kinetics					
(2-parameter)	0.381919	-2.29983	19	4.933967	2.476828
(3-parameter)	0.432099	-2.11409	20.1328	2.555188	ERR

*simultaneous biodegradation with data set #11A extracted from Table 11 on page 31 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #12A) *;

Substrate : phenol
Culture : mlss
Condition : 31C & neutral pH

Num.pts.= 14

Raw Data

S(ppm)	t(hr)
101.5	0
112.5	1
118	2
112.24	3
101.6	4
95.5	5
63	6.25
28.5	22.75
17.9	23.75
13.4	25
4.12	26.15
3	27.35
2.54	28.8
1.15	30.2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.563000	---	101.5	11.19786	142.1566
(2-parameter)	4.074454	---	115.0879	5.497992	91.27315
First-order					
(1-parameter)	0.119906	---	101.5	30.67667	548.5982
(2-parameter)	0.145767	---	204.5701	17.77639	1253.750
Monod Kinetics					
(2-parameter)	4.253354	6.193876	101.5	10.36531	155.6258
(3-parameter)	5.058611	7.684290	117.3658	4.592302	88.66798

* simultaneous biodegradation with data set #12B extracted from Table 12 on page 32 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #12B)*;

Substrate : nitrobenzene
Culture : mlss
Condition : 31C & neutral pH

Num.pts.= 14

Raw Data

S(ppm)	t(hr)
19.58	0
19.6	1
21.1	2
20.9	3
18.5	4
17.9	5
16.5	6.25
8.3	22.75
7	23.75
6.8	25
5.9	26.15
3.4	27.35
2.19	28.8
2.02	30.2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.558738	---	19.58	6.127315	1.912880
(2-parameter)	0.622448	---	21.24625	2.619198	1.014788
First-order					
(1-parameter)	0.061633	---	19.58	27.62255	7.229949
(2-parameter)	0.074046	---	27.32247	16.58279	9.485779
Monod Kinetics					
(2-parameter)	0.438265	-2.05916	19.58	5.033616	ERR
(3-parameter)	0.509970	-1.66209	20.9611	2.110781	ERR

* simultaneous biodegradation with data set #12A extracted from Table 12 on page 32 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #13A)*;

Substrate : phenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
98	0
101.6	1
96.82	2.5
93.24	4.5
89.59	6.25
80.49	7.3
3.25	22.6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.009339	---	98	6.621479	106.4390
(2-parameter)	4.615070	---	109.5350	1.812167	38.59713
First-order					
(1-parameter)	0.147145	---	98	13.19684	1102.189
(2-parameter)	0.173617	---	172.2165	4.439511	1400.981
Monod Kinetics					
(2-parameter)	1.676751	-16.6929	98	3.146463	302.9848
(3-parameter)	2.401260	-13.2386	103.3051	1.006872	147.6082

* simultaneous biodegradation with data set #13B extracted from Table 13 on page 33 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #13B)*;

Substrate : nitrobenzene
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
10.9	0
11.2	1
10.5	2.5
8.3	4.5
6.5	6.25
6.1	7.3
1.35	22.6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.483586	---	10.9	4.190652	0.980009
(2-parameter)	0.481622	---	10.87337	4.189025	0.971688
First-order					
(1-parameter)	0.090111	---	10.9	1.364848	0.876674
(2-parameter)	0.097520	---	12.28390	0.374648	0.408990
Monod Kinetics					
(2-parameter)	1.800453	14.87634	10.9	0.957505	0.486181
(3-parameter)	11.42224	112.5811	12.1224	0.367857	0.351778

* simultaneous biodegradation with data set #13A extracted from Table 13 on page 33 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #14A)*;

Substrate : phenol
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
108	0
101.6	1
98.81	2.5
83.24	4.5
79.59	6.25
60.4	7.3
3.5	22.6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	4.865872	---	108	1.202033	28.46020
(2-parameter)	4.749442	---	106.4039	1.142525	25.77217
First-order					
(1-parameter)	0.144178	---	108	5.758576	446.8258
(2-parameter)	0.164193	---	154.8649	2.193084	564.9211
Monod Kinetics					
(2-parameter)	6.495481	12.26193	108	0.549666	17.12280
(3-parameter)	7.594150	18.36110	111.3832	0.458588	17.31033

* simultaneous biodegradtion with data set #14B extracted from Table 14 on page 34 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Prasad Thesis (data set #14B) *;

Substrate : nitrobenzene
Culture : mlss
Condition : 22C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
11.9	0
11.2	1
9.5	2.5
8.7	4.5
6.75	6.25
6.1	7.3
1.35	22.6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.562642	---	11.9	5.269011	1.667993
(2-parameter)	0.488595	---	11.01021	3.900650	0.931183
First-order					
(1-parameter)	0.094855	---	11.9	0.262752	0.154418
(2-parameter)	0.097809	---	12.43447	0.142944	0.118296
Monod Kinetics					
(2-parameter)	3.940287	35.99984	11.9	0.131039	0.072483
(3-parameter)	6.057751	57.34558	12.139	0.116380	0.072545

* simultaneous biodegradation with data set #14A extracted from Table 14 on page 34 of Mr. Prasad Gonnaphula's thesis.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- McMullen Thesis (data set #1) *;

Substrate : phenol
Culture : mlss
Condition : 27C & pH 6.2-6.3

Num.pts.= 6

Raw Data

S(ppm)	t (min)
87.1	0
71	11
53.6	28
32.1	42
10.9	57
1.9	73
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k**	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.249057	---	87.1	8.012538	12.50071
(2-parameter)	1.225627	---	85.86791	7.684051	11.54270
First-order					
(1-parameter)	0.044405	---	87.1	164.9945	247.2770
(2-parameter)	0.056340	---	178.2316	80.18323	1576.435
Monod Kinetics					
(2-parameter)	1.449081	5.007720	87.1	3.319228	4.653785
(3-parameter)	1.494097	5.599445	88.1568	3.168657	4.731527

* corresponds to data extracted from Table 8 on page 63.
**units are ppm/min for zero-order & Monod and 1/min for first-order.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- McMullen Thesis (data set #1)*;

Substrate : phenol
Culture : mlss
Condition : 27C & pH 6.2-6.3

Num.pts.= 6

Raw Data

S(ppm)	t (min)
87.1	0
71	11
53.6	28
32.1	42
10.9	57
1.9	73
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 382 ppm***
Yc = -0.617***

Summary of results:

Kinetic Model	ko**	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.003478	---	6.917434	9.554108
First-order (1-parameter)	0.000129	---	183.8092	277.3466
Monod Kinetics (2-parameter)	0.003883	3.500628	4.152352	5.653591

* corresponds to data extracted from Table 8 on page 63.
** units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.
***estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- McMullen Thesis (data set #2)*;

Substrate : phenol
Culture : mlss
Condition : 27C & pH 6.0-6.3

Num.pts.= 7

Raw Data

S(ppm)	t(min)
120.1	0
95.8	11
75.2	27
51.8	43
27.6	57
3.2	69
0.8	88
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k**	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.547622	---	120.1	28.13255	67.38124
(2-parameter)	1.472935	---	115.5737	25.39483	55.09508
First-order					
(1-parameter)	0.050101	---	120.1	280.2063	645.6110
(2-parameter)	0.065650	---	362.0728	129.8246	9489.576
Monod Kinetics					
(2-parameter)	1.868206	7.294993	120.1	14.75873	14.76173
(3-parameter)	1.868003	7.292633	120.0945	14.75872	14.75755

* corresponds to data extracted from Table 9 on page 64.
**units are ppm/min for zero-order & Monod and 1/min for first-order.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- McMullen Thesis (data set #2)*;

Substrate : phenol
Culture : mlss
Condition : 27C & pH 6.0-6.3

Num.pts.= 7

Raw Data

S(ppm)	t (min)
120.1	0
95.8	11
75.2	27
51.8	43
27.6	57
3.2	69
0.8	88
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 249 ppm***
Yc = 0.335***

Summary of results:

Kinetic Model	ko**	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.005826	---	32.12615	88.41432
First-order (1-parameter)	0.000178	---	255.9289	585.1731
Monod Kinetics (2-parameter)	0.007303	9.344510	13.93117	14.44191

* corresponds to data extracted from Table 9 on page 64.
** units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.
***estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- McMullen Thesis (data set #3) *;

Substrate : o-chlorophenol
Culture : mlss
Condition : 27C & pH 7.2

Num.pts.= 9

Raw Data

S(ppm)	t (min)
24.3	0
18.4	16
14.6	30
10.5	47
5.3	76
3.9	91
2.8	106
2	121
1.4	134
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k**	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.208431	---	24.3	206.4082	8.967176
(2-parameter)	0.178310	---	21.54784	156.5160	4.976347
First-order					
(1-parameter)	0.020523	---	24.3	11.49737	0.510826
(2-parameter)	0.021420	---	26.59110	5.712664	0.722368
Monod Kinetics					
(2-parameter)	1.104464	44.03401	24.3	0.878504	0.021058
(3-parameter)	1.135341	45.41994	24.3854	0.871202	0.022358

* corresponds to data extracted from Table 30 on page 85.
**units are ppm/min for zero-order & Monod and 1/min for first-order.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- McMullen Thesis (data set #3)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : 27C & pH 7.2

Num.pts.= 9

Raw Data

S(ppm)	t(min)
24.3	0
18.4	16
14.6	30
10.5	47
5.3	76
3.9	91
2.8	106
2	121
1.4	134
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 374 ppm***
Yc = -3.214***

Summary of results:

Kinetic Model	ko**	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000610	---	172.2019	6.533304
First-order (1-parameter)	0.000063	---	25.36291	1.118551
Monod Kinetics (2-parameter)	0.002190	25.40282	0.960077	0.023848

* corresponds to data extracted from Table 30 on page 85.
** units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.
***estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- McMullen Thesis (data set #4)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : 27C & pH 6.7

Num.pts.= 7

Raw Data

S(ppm)	t(min)
22.3	0
16.1	13
12.2	30
8	46
4.9	58
2	77
1.3	90
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k **	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.272687	---	22.3	56.40295	4.194036
(2-parameter)	0.241380	---	20.37048	41.00809	2.389311
First-order					
(1-parameter)	0.029573	---	22.3	46.90007	2.296108
(2-parameter)	0.032954	---	28.12489	27.74647	6.547856
Monod Kinetics					
(2-parameter)	0.564489	10.17886	22.3	4.221786	0.332392
(3-parameter)	0.523058	9.074876	21.8727	3.976388	0.279552

* corresponds to data extracted from Table 31 on page 86.
**units are ppm/min for zero-order and Monod and 1/min for first-order.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- McMullen Thesis (data set #4) *;

Substrate : o-chlorophenol
Culture : mlss
Condition : 27C & pH 6.7

Num.pts.= 7

Raw Data

S(ppm)	t (min)
22.3	0
16.1	13
12.2	30
8	46
4.9	58
2	77
1.3	90
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 363 ppm***
Yc = -5.172***

Summary of results:

Kinetic Model	ko**	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000866	---	35.57264	2.165405
First-order (1-parameter)	0.000102	---	79.28227	3.919424
Monod Kinetics (2-parameter)	0.001408	5.518210	4.149485	0.286144

* corresponds to data extracted from Table 31 on page 86.
** units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.
***estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- McMullen Thesis (data set #5) *;

Substrate : o-chlorophenol
Culture : mlss
Condition : 28C & pH 6.6-6.7

Num.pts.= 7

Raw Data

S(ppm)	t (min)
20.9	0
17.5	17
14.3	30
13.4	50
11.5	60
9.3	75
7.2	91
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k**	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.157626	---	20.9	26.63863	0.661866
(2-parameter)	0.146999	---	20.22581	21.29056	0.460062
First-order					
(1-parameter)	0.010953	---	20.9	25.92514	0.432497
(2-parameter)	0.011406	---	21.53649	23.73892	0.508997
Monod Kinetics					
(2-parameter)	0.320292	14.94224	20.9	16.83189	0.403537
(3-parameter)	0.265567	10.55550	20.6069	16.34198	0.377334

* corresponds to extracted from Table 32 on page 87.
**units are ppm/min for zero-order & Monod and 1/min for first-order.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- McMullen Thesis (data set #5)*;

Substrate : o-chlorophenol
Culture : mlss
Condition : 28C & pH 6.6.-6.7

Num.pts.= 7

Raw Data

S(ppm)	t (min)
20.9	0
17.5	17
14.3	30
13.4	50
11.5	60
9.3	75
7.2	91
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko***	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000681	---	26.40933	0.655660
First-order (1-parameter)	0.000047	---	26.17074	0.434438
Monod Kinetics (2-parameter)	0.001366	14.56330	16.82228	0.403223

Bo = 232 ppm***
Yc = -0.106***

* corresponds to data extracted from Table 32 on page 87.
** units are ppm/ppm-min for zero-order & Monod and 1/ppm-min for first-order.
***estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #1A)*;

Substrate : phenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
97.3	0
96.1	1
86.8	2
74.4	3
52.7	5
30.2	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	9.096056	---	97.3	0.308796	25.54928
(2-parameter)	10.32894	---	103.9035	0.104628	11.16254
First-order					
(1-parameter)	0.148762	---	97.3	0.884716	94.56230
(2-parameter)	0.180212	---	116.2127	0.332982	79.08705
Monod Kinetics					
(2-parameter)	5.489560	-24.9626	97.3	0.199108	ERR
(3-parameter)	7.574595	-15.7968	102.1424	0.086687	7.322421

* simultaneous biodegradation with data sets #1B & #1C extracted from Table 3.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #1B)*;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9	0
7.8	1
6.4	2
5	3
4.3	5
3.7	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.941518	---	9	0.682172	0.604717
(2-parameter)	0.842708	---	8.561458	0.603625	0.428669
First-order					
(1-parameter)	0.145388	---	9	0.333067	0.163554
(2-parameter)	0.136980	---	8.656246	0.306235	0.151856
Monod Kinetics					
(2-parameter)	-0.63409	-10.7380	9	0.141051	0.116463
(3-parameter)	-0.51451	-9.69473	ERR	0.123698	ERR

* simultaneous biodegradation with data sets #1A & #1C extracted from Table 3.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #1C)*;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 18

Raw Data

S(ppm)	t(hr)
8.1	0
7.7	1
7.9	2
7.8	3
7	5
7.7	7
7.5	19
7.9	22
7.6	26
7.8	42
7.9	48
8	54
7.5	67
7.7	77
6.6	91
4.8	96
3.9	97
2.6	99
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.041488	---	8.1	1029.806	1.772592
(2-parameter)	0.059381	---	9.494008	666.2502	2.349279
First-order					
(1-parameter)	0.008122	---	8.1	1250.506	2.778653
(2-parameter)	0.012065	---	11.20923	722.5130	5.421691
Monod Kinetics					
(2-parameter)	0.011439	-3.94896	8.1	777.0406	1.036612
(3-parameter)	0.019812	-3.45746	8.7133	619.8855	1.119745

* simultaneous biodegradation with data sets #1A & #1B extracted from Table 3.

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Naik Thesis (data set #2A)* ;

Substrate : phenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

lum.pts.= 6

Raw Data

S(ppm)	t(hr)
100.7	0
80.5	1
58.3	2
25.2	3
5.6	5
0.2	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	17.90818	---	100.7	0.608847	195.2591
(2-parameter)	16.66868	---	95.08938	0.573283	159.2840
First-order					
(1-parameter)	0.777120	---	100.7	1.054265	465.0747
(2-parameter)	0.949355	---	265.7161	0.457732	4696.387
Monod Kinetics					
(2-parameter)	29.89792	17.54324	100.7	0.039205	16.14668
(3-parameter)	32.26897	19.58691	104.4311	0.034018	14.19708

* simultaneous biodegradation with data sets #2B & #2C extracted from Table 4 on page 22.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #2B)* ;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
8.6	0
7.8	1
5.9	2
4.7	3
3.8	5
2.4	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.992028	---	8.6	0.335755	0.330424
(2-parameter)	0.936655	---	8.343300	0.310731	0.272612
First-order					
(1-parameter)	0.179355	---	8.6	0.094369	0.096233
(2-parameter)	0.184215	---	8.809150	0.087497	0.087994
Monod Kinetics					
(2-parameter)	20.35101	108.0329	8.6	0.093745	0.094577
(3-parameter)	-13.1343	-76.1920	8.8842	0.086539	0.089927

* simultaneous biodegradation with data sets #2A & #2C extracted from Table 4 on page 22.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #2C)*;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
7.3	0
7.2	1
7.4	2
7	3
7	5
7.7	7
7.4	19
6.5	21
6.1	22
5.2	23
4.5	24
3.8	25
2.4	26
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.137284	---	7.3	82.77889	1.560136
(2-parameter)	0.204049	---	8.909288	42.84504	1.783898
First-order					
(1-parameter)	0.029199	---	7.3	104.4224	2.295640
(2-parameter)	0.045723	---	10.92198	51.11508	4.676912
Monod Kinetics					
(2-parameter)	0.041632	-3.49404	7.3	61.57920	0.979592
(3-parameter)	0.062083	-3.38471	8.0531	34.68838	0.910384

* simultaneous biodegradation with data sets #2A & #2B extracted from Table 4 on page 22.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #3A)* ;

Substrate : phenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
100.3	0
94	1
84.7	2
73.8	3
55.8	5
21.7	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	10.27707	---	100.3	0.238106	25.14840
(2-parameter)	11.30455	---	105.6303	0.134972	17.24849
First-order					
(1-parameter)	0.187978	---	100.3	1.392683	158.7212
(2-parameter)	0.233917	---	129.9204	0.680997	217.7146
Monod Kinetics					
(2-parameter)	6.202855	-23.0008	100.3	0.013536	1.562970
(3-parameter)	6.520990	-21.9890	101.2227	0.009715	0.952530

* simultaneous biodegradation with data sets #3B & #3C extracted from Table 5.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #3B)*;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9.7	0
8.2	1
7.1	2
6	3
4.8	5
3.5	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.993582	---	9.7	0.291074	0.287350
(2-parameter)	0.883275	---	9.199827	0.194612	0.151832
First-order					
(1-parameter)	0.146696	---	9.7	0.026161	0.021762
(2-parameter)	0.142745	---	9.517679	0.019707	0.016468
Monod Kinetics					
(2-parameter)	-4.32357	-36.1425	9.7	0.016699	0.008893
(3-parameter)	-5.36876	-43.6300	9.6273	0.016230	0.009189

* simultaneous biodegradation with data sets #3A & #3C extracted from Table 5.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #3C)*;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 18

Raw Data

S(ppm)	t(hr)
8.7	0
7.9	1
7.9	2
8.2	3
7.8	5
7.7	7
7.9	19
7.8	22
8.1	26
8	42
7.9	48
8.1	54
7.9	67
7.7	77
6.5	91
4.6	96
3.5	97
2.3	99
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.048274	---	8.7	760.8869	1.773204
(2-parameter)	0.063723	---	9.815264	591.7872	2.403040
First-order					
(1-parameter)	0.009346	---	8.7	1053.149	3.045668
(2-parameter)	0.013450	---	11.98627	675.7426	6.573213
Monod Kinetics					
(2-parameter)	0.016130	-3.72522	8.7	516.8474	1.177402
(3-parameter)	0.019033	-3.56531	8.8849	507.1387	1.157618

* simultaneous biodegradation with data sets #3A & #3B extracted from Table 5.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #4A)* ;

Substrate : phenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
99.3	0
81.7	1
50.2	2
27.4	3
7.8	5
0.4	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	17.58161	---	99.3	0.624532	193.0512
(2-parameter)	16.19153	---	93.04125	0.578615	151.6931
First-order					
(1-parameter)	0.688051	---	99.3	0.921738	313.7445
(2-parameter)	0.829313	---	217.5014	0.426695	2388.223
Monod Kinetics					
(2-parameter)	30.48418	21.05696	99.3	0.035350	12.27944
(3-parameter)	32.09587	22.65019	101.6529	0.033184	10.72950

* simultaneous biodegradation with data sets #4B & #4C extracted from Table 6.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #4B)*;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9.3	0
8.2	1
6	2
4.5	3
3.1	5
2	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.217562	---	9.3	0.403194	0.597719
(2-parameter)	1.135410	---	8.922899	0.367557	0.473839
First-order					
(1-parameter)	0.221488	---	9.3	0.044857	0.107113
(2-parameter)	0.226721	---	9.544078	0.039592	0.088189
Monod Kinetics					
(2-parameter)	-30.9206	-144.971	9.3	0.044354	0.113944
(3-parameter)	-6.39479	-32.9580	9.876	0.032303	0.126543

* simultaneous biodegradation with data sets #4A & #4C extracted from Table 6.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #4C) *;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 25C & neutral pH

Num.pts.= 13

Raw Data

S(ppm)	t(hr)
7.9	0
8	1
8.1	2
7.9	3
7.8	5
8	7
7.9	19
6.6	21
6	22
5.3	23
4.2	24
3.4	25
2.1	26
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.165958	---	7.9	68.14675	1.876919
(2-parameter)	0.236568	---	9.639164	33.93281	1.899033
First-order					
(1-parameter)	0.034971	---	7.9	93.66637	2.996199
(2-parameter)	0.053071	---	12.37092	45.17932	6.160307
Monod Kinetics					
(2-parameter)	0.055333	-3.40183	7.9	46.84371	1.281584
(3-parameter)	0.076231	-3.35475	8.7011	23.77503	1.129769

* simultaneous biodegradation with data sets #4A & #4B extracted from Table 6.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #5A) *;

Substrate : phenol
Culture : phenol-acclimated sludge
Condition : 25C & neutral pH

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
100	0
84.5	0.5
55.3	1
8.7	1.5
1	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	52.59429	---	100	0.026836	74.23384
(2-parameter)	57.15836	---	107.0583	0.020979	68.54327
First-order					
(1-parameter)	2.033216	---	100	0.167164	826.4827
(2-parameter)	2.674567	---	304.3477	0.070630	8593.456
Monod Kinetics					
(2-parameter)	55.67098	1.683620	100	0.026296	68.95630
(3-parameter)	69.92439	5.517143	110.6596	0.017825	62.53078

* simultaneous biodegradation with data sets #5B & #5C extracted from Table 7.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #5B)*;

Substrate : nitrobenzene
Culture : phenol-acclimated sludge
Condition : 25C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
10	0
9.4	0.5
9.6	1
10	1.5
9.6	2
8.7	2.5
8.4	3
7.4	4
6.7	5
4.9	6
4.4	7
2.4	8
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.824363	---	10	0.842410	0.572481
(2-parameter)	0.988146	---	10.95999	0.362493	0.353950
First-order					
(1-parameter)	0.137390	---	10	2.155937	1.742451
(2-parameter)	0.179518	---	13.00213	0.874966	1.846968
Monod Kinetics					
(2-parameter)	0.447680	-2.89764	10	0.482488	ERR
(3-parameter)	0.603190	-2.28648	10.5733	0.266507	ERR

* simultaneous biodegradation with data sets #5A & #5C extracted from Table 7.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #5C) *;

Substrate : 2,6-dichlorophenol
Culture : phenol-acclimated sludge
Condition : 25C & neutral pH

Num.pts.= 18

Raw Data

S(ppm)	t(hr)
8.5	0
9.3	0.5
8.7	1
9.6	1.5
9.5	2
9.3	2.5
9.4	3
9.2	4
9.2	5
9.5	6
9.2	7
9	8
9.3	20
9.3	23
9.4	24
6.1	26
3.2	28
1.5	29
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.280787	---	8.5	158.4362	12.49136
(2-parameter)	0.317283	---	11.64680	60.92803	6.133543
First-order					
(1-parameter)	0.054667	---	8.5	145.4104	12.37436
(2-parameter)	0.069822	---	16.08517	65.62941	19.19439
Monod Kinetics					
(2-parameter)	-0.20104	-8.24788	8.5	139.1981	18.58435
(3-parameter)	0.177265	-2.14568	10.9194	59.73697	3.790883

* simultaneous biodegradation with data sets #5A & #5B extracted from Table 7.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #6A)*;

Substrate : phenol
Culture : phenol-acclimated sludge
Condition : 25C & neutral pH

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
94	0
78.8	0.5
49.1	1
10.8	1.5
1.3	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	48.97320	---	94	0.018781	45.04562
(2-parameter)	52.27608	---	99.07608	0.015265	41.71854
First-order					
(1-parameter)	1.870135	---	94	0.158373	596.1461
(2-parameter)	2.443596	---	252.8488	0.068290	5201.405
Monod Kinetics					
(2-parameter)	52.92472	2.354526	94	0.017752	41.55334
(3-parameter)	63.92580	5.558569	102.1997	0.011873	35.95173

* simultaneous biodegradation with data sets #6B &6C extracted from Table 8.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #6B)*;

Substrate : nitrobenzene
Culture : phenol-acclimated sludge
Condition : 25C & neutral pH

Num.pts.= 12

Raw Data

S(ppm)	t(hr)
10.5	0
10.1	0.5
9.9	1
10	1.5
9.6	2
8.9	2.5
8.6	3
7.4	4
6.3	5
4.9	6
3.7	7
2.1	8
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.940005	---	10.5	0.455324	0.402329
(2-parameter)	1.083978	---	11.32509	0.180669	0.212288
First-order					
(1-parameter)	0.157258	---	10.5	1.807303	1.849040
(2-parameter)	0.201894	---	13.82401	0.729827	2.051302
Monod Kinetics					
(2-parameter)	0.569914	-2.49438	10.5	0.196828	ERR
(3-parameter)	0.709233	-1.98875	10.9524	0.102240	ERR

* simultaneous biodegradation with data sets #6A & #6C extracted from Table 8.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #6C)*;

Substrate : 2,6-dichlorophenol
Culture : phenol-acclimated sludge
Condition : 25C & neutral pH

Num.pts.= 18

Raw Data

S(ppm)	t(hr)
8.7	0
8.8	0.5
8.7	1
8.6	1.5
8.7	2
8.6	2.5
8.7	3
8.6	4
8.6	5
8.6	6
8.5	7
8.2	8
8.2	20
8.4	23
8.3	24
5.7	26
2.4	28
1.7	29
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.200631	---	8.7	87.26253	3.512567
(2-parameter)	0.269520	---	10.51909	50.59374	3.675206
First-order					
(1-parameter)	0.045895	---	8.7	104.1847	6.187599
(2-parameter)	0.063021	---	13.86741	58.25049	11.29282
Monod Kinetics					
(2-parameter)	0.047528	-3.59601	8.7	62.65973	2.255615
(3-parameter)	0.067093	-3.46826	9.3069	40.24882	2.058307

* simultaneous biodegradation with data sets #6A & #6B extracted from Table 8.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #7A)*;

Substrate : 2-chlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
20.5	0
18.6	1
15.9	2
14.7	3
13.2	4
11.8	5
10.7	6
10.1	7
7	22
5.5	27
4.3	33
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.722253	---	20.5	37.04869	19.32648
(2-parameter)	0.505436	---	17.08164	25.34195	6.474021
First-order					
(1-parameter)	0.055155	---	20.5	14.84256	6.537912
(2-parameter)	0.044693	---	16.98304	8.460617	3.060336
Monod Kinetics					
(2-parameter)	-0.45858	-20.5151	20.5	2.146695	0.791270
(3-parameter)	-0.43790	-19.9724	ERR	2.123034	ERR

* simultaneous biodegradation with data sets #7B & #7C extracted from Table 9.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #7B)* ;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
7.1	0
6.2	1
5	2
4.7	3
3.9	4
3.2	5
2.8	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.780113	---	7.1	0.108105	0.065790
(2-parameter)	0.73	---	6.89	0.086105	0.045885
First-order					
(1-parameter)	0.154671	---	7.1	0.033847	0.017926
(2-parameter)	0.157084	---	7.174935	0.032438	0.018199
Monod Kinetics					
(2-parameter)	4.987338	27.23635	7.1	0.031226	0.017325
(3-parameter)	5.529987	30.63073	7.1145	0.031191	0.017380

* simultaneous biodegradation with data sets #7A & #7C extracted from Table 9.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #7C)*;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 19

Raw Data

S(ppm)	t(hr)
8.3	0
8.3	1
8.1	2
7.9	3
8.3	4
8.2	5
8.1	6
8.4	7
8.1	22
8.3	27
8.6	33
8.7	44
8.5	49
8.4	57
8.4	68
7.8	70
6.6	73
3.5	76
1.1	79
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.074892	---	8.3	1204.173	6.754137
(2-parameter)	0.116455	---	11.39479	591.9280	8.027660
First-order					
(1-parameter)	0.020285	---	8.3	1315.907	12.20369
(2-parameter)	0.031891	---	20.09035	630.4904	49.68160
Monod Kinetics					
(2-parameter)	0.032742	-2.30610	8.3	1148.872	3.368582
(3-parameter)	0.056433	-2.08646	10.194	577.0148	3.942102

* simultaneous biodegradation with data sets #7A & #7B extracted from Table 9.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #8A)*;

Substrate : 2-chlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
18.4	0
15.4	1
12.9	2
10.1	3
6.9	4
4.2	5
2.6	6
1.3	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.656803	---	18.4	0.073042	0.515580
(2-parameter)	2.567464	---	17.96112	0.064924	0.427971
First-order					
(1-parameter)	0.327706	---	18.4	0.606741	3.823308
(2-parameter)	0.391962	---	26.03626	0.276373	8.877750
Monod Kinetics					
(2-parameter)	3.481747	2.635150	18.4	0.012148	0.109641
(3-parameter)	3.665251	3.021784	18.664	0.010687	0.072043

* simultaneous biodegradation with data sets #8B & #8C extracted from Table 10.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #8B)*;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
9.3	0
8.2	1
6.9	2
5.7	3
4.7	4
3.4	5
2.1	6
1.2	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.175379	---	9.3	0.005656	0.007815
(2-parameter)	1.176266	---	9.304432	0.005652	0.007820
First-order					
(1-parameter)	0.247789	---	9.3	0.744420	0.786646
(2-parameter)	0.300099	---	12.34269	0.363913	1.514655
Monod Kinetics					
(2-parameter)	1.206104	0.129615	9.3	0.005128	0.006817
(3-parameter)	1.229881	0.192433	9.3436	0.004846	0.006452

* simultaneous biodegradation with data sets #8A & #8C extracted from Table 10.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #8C)*;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
8.3	0
7.7	1
8.1	2
7.9	3
8.4	4
8.2	5
8.1	6
8	7
7.9	22
7.1	23
6.2	25
5.3	26
4.2	27
3.1	28
1.9	29
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.163623	---	8.3	70.20185	1.879479
(2-parameter)	0.220579	---	9.752036	43.55886	2.119371
First-order					
(1-parameter)	0.034780	---	8.3	103.8449	3.226772
(2-parameter)	0.050517	---	12.55779	57.68581	6.659998
Monod Kinetics					
(2-parameter)	0.054939	-3.40626	8.3	42.25134	1.404490
(3-parameter)	0.072646	-3.26381	8.842	31.25375	1.277718

* simultaneous biodegradation with data sets #8A & #8B extracted from Table 10.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #9A)* ;

Substrate : 2-chlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
19.6	0
18.3	1
15.7	2
14.8	3
13.5	4
11.5	5
10.3	6
9.4	7
7	22
5.6	27
4.1	33
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.671561	---	19.6	34.87854	15.73006
(2-parameter)	0.494106	---	16.74106	25.53568	6.234312
First-order					
(1-parameter)	0.053720	---	19.6	14.49138	5.359554
(2-parameter)	0.045026	---	16.71778	9.749246	2.958827
Monod Kinetics					
(2-parameter)	-0.46727	-20.4081	19.6	4.065799	1.045544
(3-parameter)	-0.44116	-19.7274	ERR	4.030865	ERR

* simultaneous biodegradation with data sets #9B & #9C extracted from Table 11.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #9B)* ;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 7

Raw Data

S(ppm)	t(hr)
8.1	0
7.2	1
5.7	2
4.5	3
3.8	4
3.1	5
2.5	6
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.022535	---	8.1	0.104879	0.109660
(2-parameter)	0.984705	---	7.939830	0.097454	0.094496
First-order					
(1-parameter)	0.192369	---	8.1	0.028589	0.044322
(2-parameter)	0.201399	---	8.429995	0.015353	0.031592
Monod Kinetics					
(2-parameter)	4.153205	16.32047	8.1	0.019596	0.026839
(3-parameter)	10.23099	46.02263	8.344	0.014435	0.024928

* simultaneous biodegradation with data sets #9A & #9C extracted from Table 11.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #9C)* ;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 19

Raw Data

S(ppm)	t(hr)
8.6	0
8.5	1
8.4	2
8.5	3
8.3	4
8.6	5
8.2	6
8.4	7
8.7	22
8.4	27
8.6	33
8.7	44
8.5	49
8.5	57
8.4	68
7.8	70
6.7	73
3.8	76
1.4	79
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.068792	---	8.6	1056.731	5.000908
(2-parameter)	0.106109	---	11.23285	550.5479	6.198702
First-order					
(1-parameter)	0.017272	---	8.6	1229.167	9.832323
(2-parameter)	0.027164	---	17.80298	606.2212	32.67928
Monod Kinetics					
(2-parameter)	0.021373	-3.11778	8.6	888.7513	2.240918
(3-parameter)	0.036604	-2.88605	9.8041	505.6305	2.454720

* simultaneous biodegradation with data sets #9A & #9B extracted from Table 11.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #10A)*;

Substrate : 2-chlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
19.6	0
16.4	1
13.7	2
11	3
7.2	4
4.5	5
2.3	6
1.1	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	2.861523	---	19.6	0.061734	0.505497
(2-parameter)	2.784745	---	19.22160	0.056526	0.438350
First-order					
(1-parameter)	0.352032	---	19.6	0.808455	5.972618
(2-parameter)	0.431577	---	30.26015	0.362819	17.11052
Monod Kinetics					
(2-parameter)	3.531673	2.016927	19.6	0.014973	0.105466
(3-parameter)	3.703264	2.337434	19.887	0.013373	0.103698

* simultaneous biodegradation with data sets #10B & #10C extracted from Table 12.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #10B) *;

Substrate : nitrobenzene
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
8.9	0
8.2	1
6.5	2
5.5	3
4.2	4
3.3	5
2	6
1.4	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	1.119693	---	8.9	0.039858	0.049970
(2-parameter)	1.132203	---	8.962711	0.038922	0.049893
First-order					
(1-parameter)	0.235300	---	8.9	0.488053	0.554281
(2-parameter)	0.277095	---	11.13958	0.218953	0.761961
Monod Kinetics					
(2-parameter)	1.272451	0.669108	8.9	0.031054	0.038475
(3-parameter)	1.445955	1.189446	9.1424	0.022880	0.030693

* simultaneous biodegradation with data sets #10A & #10C extracted from Table 12.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #10C)*;

Substrate : 2,6-dichlorophenol
Culture : unacclimated sludge
Condition : 27C & neutral pH

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
9.3	0
8.7	1
8.9	2
8.9	3
9	4
8.8	5
8.9	6
8.8	7
8.9	22
8.1	23
7	25
5.7	26
4.5	27
3.3	28
1.7	29
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.192392	---	9.3	71.84016	2.659150
(2-parameter)	0.259892	---	10.97050	47.30081	3.194885
First-order					
(1-parameter)	0.039339	---	9.3	111.7327	4.892775
(2-parameter)	0.058323	---	15.20294	62.84236	12.23303
Monod Kinetics					
(2-parameter)	0.072315	-3.39644	9.3	44.69114	1.958201
(3-parameter)	0.095123	-3.21504	9.91	36.01829	1.854714

* simultaneous biodegradation with data sets #10A & #10B extracted from Table 12.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #11B)* ;

Substrate : nitrobenzene
Culture : phenol-acclimated sludge
Condition : 27C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
7	0
4.8	0.25
4.2	0.5
3.6	1
1.9	1.5
0.7	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.513281	---	7	0.045977	0.567505
(2-parameter)	2.972809	---	6.301208	0.030864	0.272769
First-order					
(1-parameter)	1.035900	---	7	0.041514	0.303075
(2-parameter)	1.114204	---	7.852899	0.036886	0.561943
Monod Kinetics					
(2-parameter)	7.295563	3.770755	7	0.022972	0.325798
(3-parameter)	5.204338	2.134510	6.5578	0.020534	0.242681

* simultaneous biodegradation with data sets #11A & #11C extracted from Table 13.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #11C)*;

Substrate : 2,6-dichlorophenol
Culture : phenol-acclimated sludge
Condition : 27C & neutral pH

Num.pts.= 16

Raw Data

S(ppm)	t(hr)
8.9	0
8.8	0.25
8.5	0.5
8.6	1
8.8	1.5
8.8	2
8.4	4
8.8	6
8.6	9
8.8	22
8.6	26
8.2	28
7.6	30
5.9	32
2.9	34
1.3	36
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.162976	---	8.9	155.1395	4.120722
(2-parameter)	0.227158	---	10.89109	98.15956	5.065136
First-order					
(1-parameter)	0.039936	---	8.9	201.2577	8.173038
(2-parameter)	0.058221	---	16.17914	115.8518	24.99725
Monod Kinetics					
(2-parameter)	0.053264	-3.10254	8.9	114.1121	2.424689
(3-parameter)	0.077399	-2.90979	9.6825	83.53555	2.390878

* simultaneous biodegradation with data sets #11A & #11B extracted from Table 13.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #12B)* ;

Substrate : nitrobenzene
Culture : phenol-acclimated sludge
Condition : 27C & neutral pH

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
7.9	0
5.8	0.25
4.2	0.5
3.8	1
2.9	1.5
1.5	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.767320	---	7.9	0.075887	1.07705
(2-parameter)	3.103533	---	7.065591	0.057789	0.556625
First-order					
(1-parameter)	0.805709	---	7.9	0.029405	0.328815
(2-parameter)	0.770119	---	7.523401	0.028012	0.257539
Monod Kinetics					
(2-parameter)	-45.6999	-61.2314	7.9	0.029143	0.295391
(3-parameter)	47.84130	58.36683	7.4505	0.027878	0.270353

* simultaneous biodegradation with data sets #12A & #12C extracted from Table 14.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Naik Thesis (data set #12C)*;

Substrate : 2,6-dichlorophenol
Culture : phenol-acclimated sludge
Condition : 27C & neutral pH

Num.pts.= 16

Raw Data

S(ppm)	t(hr)
7.9	0
7.9	0.25
8	0.5
8.1	1
7.8	1.5
8.2	2
8.1	4
8	6
7.9	9
7.8	22
7.6	26
7.2	28
5.8	30
4.9	32
3	34
1	36
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.142676	---	7.9	140.2959	2.855952
(2-parameter)	0.191370	---	9.602857	78.17644	2.863019
First-order					
(1-parameter)	0.040931	---	7.9	196.8793	6.303868
(2-parameter)	0.058100	---	14.41952	107.6878	18.00496
Monod Kinetics					
(2-parameter)	0.058009	-2.40330	7.9	106.5933	1.727494
(3-parameter)	0.075330	-2.39674	8.7398	59.02954	1.602217

* simultaneous biodegradation with data sets #12A & #12B extracted from Table 14.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #1)* ;

Substrate : 2,6-dichlorophenol
Culture : mlss (acclimated sludge)
Condition : 23C & pH 7.5-7.6

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
9.59	0
8.99	2
8.76	4
8.44	6
8.37	8
6.96	23
6.9	25
6.87	27
6.56	29
5.88	31
0.08	47
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.159131	---	9.59	48.44946	1.226881
(2-parameter)	0.188185	---	10.49213	37.34534	1.322538
First-order					
(1-parameter)	0.085090	---	9.59	249.6165	16.68944
(2-parameter)	0.128862	---	53.81297	104.7477	369.9849
Monod Kinetics					
(2-parameter)	0.099495	-1.00907	9.59	6.191295	1.507085
(3-parameter)	0.086566	-1.08023	9.2841	3.703227	1.743724

* corresponds to data extracted from Table 16 on page 39.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #1) *;

Substrate : 2,6-dichlorophenol
Culture : mlss (acclimated sludge)
Condition : 23C & pH 7.5-7.6

Num.pts.= 11

Raw Data

S(ppm)	t(hr)
9.59	0
8.99	2
8.76	4
8.44	6
8.37	8
6.96	23
6.9	25
6.87	27
6.56	29
5.88	31
0.08	47
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Bo = 4250 ppm **
Yc = -41.3 **

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000039	---	53.12666	1.320622
First-order (1-parameter)	0.000021	---	255.2972	17.28635
Monod Kinetics (2-parameter)	0.000023	-1.01247	6.038392	1.561244

* corresponds to data extracted from Table 16 on page 39.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #2)*;

Substrate : 2,6-dichlorophenol
Culture : mlss (acclimated sludge)
Condition : 24C & pH 7.3-7.4

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
9.41	0
8.99	2
8.91	4
8.71	6
7.52	10
1.35	23
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.328658	---	9.41	7.003738	0.756518
(2-parameter)	0.378508	---	10.32047	3.076351	0.440743
First-order					
(1-parameter)	0.080366	---	9.41	15.29876	4.112662
(2-parameter)	0.096886	---	13.16876	6.140886	4.294128
Monod Kinetics					
(2-parameter)	0.116530	-2.77150	9.41	0.904114	2.185617
(3-parameter)	0.131122	-2.64349	9.5315	0.742969	1.760721

* corresponds to data extracted from Table 17 on page 39.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #3)*;

Substrate : 2,6-dichlorophenol
Culture : mlss (unacclimated sludge)
Condition : 25C & pH 7.9-8.1

Num.pts.= 20

Raw Data

S(ppm)	t(hr)
10.83	0
10.59	2
10.13	4
9.66	6
9.04	8
8.22	24
8.11	26
7.58	28
7.46	30
6.73	32
5.24	48
5.27	50
5.25	52
4.91	54
4.77	56
4.2	72
3.98	74
3.54	76
3.35	78
2.46	80
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.103428	---	10.83	22.94821	0.245485
(2-parameter)	0.095454	---	10.38416	17.21855	0.156885
First-order					
(1-parameter)	0.014974	---	10.83	32.44005	0.156949
(2-parameter)	0.015821	---	11.38486	29.05011	0.209786
Monod Kinetics					
(2-parameter)	0.167916	4.354853	10.83	16.72815	0.131351
(3-parameter)	0.130604	2.282173	10.5251	15.28118	0.118479

* corresponds to data extracted from Table 12 on page 37.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #3)*;

Substrate : 2,6-dichlorophenol
Culture : mlss (unacclimated sludge)
Condition : 25C & pH 7.9-8.1

Num.pts.= 20

Raw Data

S(ppm)	t(hr)
10.83	0
10.59	2
10.13	4
9.66	6
9.04	8
8.22	24
8.11	26
7.58	28
7.46	30
6.73	32
5.24	48
5.27	50
5.25	52
4.91	54
4.77	56
4.2	72
3.98	74
3.54	76
3.35	78
2.46	80
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000027	---	20.96710	0.217376
First-order (1-parameter)	0.000004	---	36.18287	0.172644
Monod Kinetics (2-parameter)	0.000041	3.278566	16.47538	0.130955

Bo = 3830 ppm **
Yc = -36.5 **

* corresponds to data extracted from Table 12 on page 37.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #4)*;

Substrate : 2,6-dichlorophenol
Culture : mlss (unacclimated sludge)
Condition : 23C & pH 6.7-6.9

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
9.62	0
8.73	2
8.43	4
7.36	6
6.56	8
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.374145	---	9.62	0.169689	0.023753
(2-parameter)	0.382336	---	9.669345	0.163969	0.023969
First-order					
(1-parameter)	0.045465	---	9.62	0.281582	0.037628
(2-parameter)	0.048242	---	9.785092	0.235731	0.038415
Monod Kinetics					
(2-parameter)	0.208828	-3.64794	9.62	0.142483	0.019116
(3-parameter)	0.196432	-3.87747	9.5999	0.141658	0.018595

* corresponds to data extracted from Table 13 on page 37.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #5)* ;

Substrate : 2-chlorophenol
Culture : mlss (acclimated sludge)
Condition : 25C & pH 7.8-8.0

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
19.91	0
14	0.58
5.72	1.03
2.86	1.5
2.02	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	10.66819	---	19.91	0.040951	4.660719
(2-parameter)	10.41828	---	19.54948	0.040610	4.407910
First-order					
(1-parameter)	1.189905	---	19.91	0.020806	3.279891
(2-parameter)	1.287362	---	23.13434	0.015859	4.020313
Monod Kinetics					
(2-parameter)	40.80988	25.51439	19.91	0.018012	1.877490
(3-parameter)	125.2370	89.65602	22.2885	0.015666	2.827105

* corresponds to data extracted from Table 9 on page 35.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #5)*;

Substrate : 2-chlorophenol
Culture : mlss (acclimated sludge)
Condition : 25C & pH 7.8-8.0

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
19.91	0
14	0.58
5.72	1.03
2.86	1.5
2.02	2
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.002776	---	0.040238	4.393991
First-order (1-parameter)	0.000312	---	0.021299	3.433923
Monod Kinetics (2-parameter)	0.009989	23.28703	0.018112	1.901152

Bo = 3920 ppm **
Yc = -9.6 **

* corresponds to data extracted from Table 9 on page 35.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #6)*;

Substrate : 2-chlorophenol
Culture : mlss (acclimated sludge)
Condition : 23C & pH 7.8-8.0

Num.pts.= 5

Raw Data

S(ppm)	t(hr)
18.56	0
13.37	0.53
7.84	1.05
3.19	1.5
1.72	2.05
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	9.243403	---	18.56	0.018319	1.565246
(2-parameter)	8.939534	---	18.10796	0.017552	1.402703
First-order					
(1-parameter)	1.117834	---	18.56	0.029120	2.834025
(2-parameter)	1.255839	---	23.18747	0.016274	5.263624
Monod Kinetics					
(2-parameter)	15.73214	5.950103	18.56	0.006888	0.320648
(3-parameter)	18.04440	7.553869	19.1607	0.006372	0.334357

* corresponds to data extracted from Table 10 on page 35.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #7)*;

Substrate : 2-chlorophenol
Culture : mlss (unacclimated sludge)
Condition : 22C & pH 7.4-8.0

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
18.49	0
16.5	2
15.58	4
14.44	6
8.77	20
7.77	22
6.75	24
6.41	26
5.76	28
5.68	30
3.66	46
3	48
2.93	50
2.6	52
2.08	54.25
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.361778	---	18.49	40.86991	5.349212
(2-parameter)	0.304166	---	16.38749	30.95141	2.863530
First-order					
(1-parameter)	0.038452	---	18.49	2.841515	0.118965
(2-parameter)	0.037704	---	17.95291	2.659731	0.094932
Monod Kinetics					
(2-parameter)	-4.51264	-126.460	18.49	2.637250	0.081260
(3-parameter)	-6.76925	-186.950	18.1925	2.611376	0.076964

* corresponds to data extracted from Table 6 on page 33.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #7)*;

Substrate : 2-chlorophenol
Culture : mlss (unacclimated sludge)
Condition : 22C & pH 7.4-8.0

Num.pts.= 15

Raw Data

S(ppm)	t(hr)
18.49	0
16.5	2
15.58	4
14.44	6
8.77	20
7.77	22
6.75	24
6.41	26
5.76	28
5.68	30
3.66	46
3	48
2.93	50
2.6	52
2.08	54.25
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000085	---	43.84690	6.170249
First-order (1-parameter)	0.000008	---	3.259970	0.168895
Monod Kinetics (2-parameter)	-0.00059	-76.0320	2.632051	0.080671

Bo = 4064 ppm**
Yc = 27.3**

* corresponds to data extracted from Table 6 on page 33.
**estimated from available MLSS measurements.

egression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

ata source -- Pak Thesis (data set #8)*;

Substrate : 2-chlorophenol
Culture : mlss (unacclimated sludge)
Condition : 23C & pH 8.0-8.1

um.pts.= 6

Raw Data

S(ppm)	t(hr)
21.01	0
15.32	2
10.44	4
3.17	20
2.12	22
0.45	24
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.941213	---	21.01	13.01792	11.53235
(2-parameter)	0.778959	---	18.09918	9.191561	5.577238
First-order					
(1-parameter)	0.131545	---	21.01	13.59504	1.407241
(2-parameter)	0.140092	---	24.99931	12.92251	7.869924
Monod Kinetics					
(2-parameter)	1.793228	6.801985	21.01	7.734906	6.753772
(3-parameter)	1.240614	3.706206	18.5203	6.416380	4.339864

* corresponds to data extracted from Table 6 on page 33.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #9)*;

Substrate : phenol
Culture : mlss
Condition : 22C & pH 7.5-7.8

Num.pts.= 10

Raw Data

S(ppm)	t(hr)
99.09	0
96.76	1
94.48	2
91.48	3
86.22	4
82.67	5
76.66	6
67.93	7.42
10.66	22.75
7.54	24
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	3.836432	---	99.09	0.338466	4.981624
(2-parameter)	3.950997	---	101.0486	0.196654	3.069852
First-order					
(1-parameter)	0.100042	---	99.09	5.308543	238.8508
(2-parameter)	0.112848	---	128.1490	1.643398	162.6015
Monod Kinetics					
(2-parameter)	3.680577	-1.62050	99.09	0.329933	4.748510
(3-parameter)	4.601405	5.916001	102.257	0.155073	2.869140

* corresponds to data extracted from Table 1 on page 31.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Pak Thesis (data set #9)* ;

Substrate : phenol
Culture : mlss
Condition : 22C & pH 7.5-7.8

Num.pts.= 10

Raw Data

S(ppm)	t(hr)
99.09	0
96.76	1
94.48	2
91.48	3
86.22	4
82.67	5
76.66	6
67.93	7.42
10.66	22.75
7.54	24
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.001025	---	0.440784	7.136757
First-order (1-parameter)	0.000027	---	5.956465	290.4399
Monod Kinetics (2-parameter)	0.000906	-4.47746	0.362396	ERR

Bo = 4026 ppm **
Yc = -6.6 **

* corresponds to data extracted from Table 1 on page 31.
**estimated from available MLSS measurements.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Pak Thesis (data set #10)*;

Substrate : phenol
Culture : mlss
Condition : 21C & pH 7.5-7.8

Num.pts.= 8

Raw Data

S(ppm)	t(hr)
104.59	0
85.22	1
60.49	2
22.12	3
6.62	4
4.78	5
4.05	6
0.79	7
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	19.24262	---	104.59	0.767942	284.3525
(2-parameter)	18.27717	---	100.0526	0.752998	251.5430
First-order					
(1-parameter)	0.630804	---	104.59	0.431158	234.1883
(2-parameter)	0.726848	---	173.8060	0.240915	650.6284
Monod Kinetics					
(2-parameter)	48.05863	47.31678	104.59	0.199597	48.51679
(3-parameter)	67.40770	71.35433	118.101	0.176656	52.89244

* corresponds to data extracted from Table 2 on page 31.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Constant Biomass Assumed

Data source -- Salerno Thesis (data set #1)* ;

Substrate : 2,4-dichlorophenol
Culture : mlss
Condition : 23C & pH 7.4-7.5

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
11.5	0
11.1	90
8.8	180
8.3	280
8.2	365
7.2	455
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	k	K	So	avg dt^2	avg dS^2
Zero-order					
(1-parameter)	0.010279	---	11.5	2283.653	0.241311
(2-parameter)	0.010581	---	11.59937	2255.794	0.252562
First-order					
(1-parameter)	0.001070	---	11.5	1909.798	0.190356
(2-parameter)	0.001118	---	11.68810	1840.353	0.194240
Monod Kinetics					
(2-parameter)	-0.00800	-17.0479	11.5	1737.245	0.190925
(3-parameter)	-0.00510	-13.9138	12.4399	1495.717	0.301882

*corresponds to data extracted from Table 35 on page 82.

Regression of Batch-Reactor Biodegradation Data (with respect to time) : Variable Biomass

Data source -- Salerno Thesis (data set #1)*;

Substrate : 2,4-dichlorophenol
Culture : mlss
Condition : 23C & pH 7.4-7.5

Num.pts.= 6

Raw Data

S(ppm)	t(hr)
11.5	0
11.1	90
8.8	180
8.3	280
8.2	365
7.2	455
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA
NA	NA

Summary of results:

Kinetic Model	ko	K	avg dt^2	avg dS^2
Zero-order (1-parameter)	0.000061	---	2249.527	0.235119
First-order (1-parameter)	0.000006	---	1887.759	0.188466
Monod Kinetics (2-parameter)	-0.00005	-17.5957	1735.872	0.190494

Bo = 169 ppm**
Yc = -1.45 **

* corresponds to data extracted from Table 35 on page 82.
**estimated from available MLSS measurements.

Appendix F

Compilation of Analysis Results from the Study of the Effect of Experimental Error in Biodegradation Data on Kinetic Model Selection

Table of Contents

Tabulation of Ideal S vs. t Data

(Constant-Biomass Behavior Assumed)*

S(ppm)	t(hr)	S(ppm)	t(hr)	S(ppm)	t(hr)	S(ppm)	t(hr)	S(ppm)	t(hr)
100.00	0	65.05	149.40	33.61	298.80	10.25	448.20	1.23	597.60
98.20	7.47	63.37	156.87	32.20	306.27	9.44	455.67	1.08	605.07
96.41	14.94	61.70	164.34	30.80	313.74	8.67	463.14	0.95	612.54
94.62	22.41	60.04	171.81	29.42	321.21	7.94	470.61	0.84	620.01
92.83	29.88	58.39	179.28	28.07	328.68	7.21	478.08	0.74	627.48
91.05	37.35	56.75	186.75	26.73	336.15	6.60	485.55	0.65	634.95
89.28	44.82	55.12	194.22	25.43	343.62	6.00	493.02	0.57	642.42
87.51	52.29	53.50	201.69	24.14	351.09	5.43	500.49	0.50	649.89
85.74	59.76	51.89	209.16	22.88	358.56	4.98	507.96	0.44	657.36
83.98	67.23	50.29	216.63	21.65	366.03	4.42	515.43	0.38	664.83
82.23	74.70	48.71	224.10	20.45	373.50	3.98	522.90	0.34	672.30
80.48	82.17	47.13	231.57	19.28	380.97	3.57	530.37	0.29	679.77
78.74	89.64	45.57	239.04	18.14	388.44	3.19	537.84	0.26	687.24
77.00	97.11	44.02	246.51	17.03	395.91	2.85	545.31	0.23	694.71
75.27	104.58	42.49	253.98	15.95	403.38	2.54	552.78	0.20	702.18
73.55	112.05	40.97	261.45	14.91	410.85	2.26	560.25	0.18	709.65
71.83	119.52	39.47	268.92	13.90	418.32	2.00	567.72	0.16	717.12
70.13	126.99	37.98	276.39	12.97	425.79	1.78	575.19	0.14	724.59
68.45	134.46	36.41	283.86	12.01	433.26	1.57	582.66	0.12	732.06
66.73	141.93	35.05	291.33	11.10	440.73	1.39	590.13	0.10	739.53

---

* Refer to Figure 104: data derived using the M2 model with k = 0.278 ppm/hr., K = 15.3 ppm and So = 100 ppm!

Tabulation of Ideal S vs. t Data

(Variable-Biomass Behavior Assumed)*

S(ppm)	t(hr)	S(ppm)	t(hr)	S(ppm)	t(hr)	S(ppm)	t(hr)	S(ppm)	t(hr)
100.00	0	96.97	7.336	88.83	14.672	67.71	22.008	21.77	29.344
99.91	0.367	96.73	7.703	88.18	15.039	66.07	22.375	19.09	29.711
99.81	0.734	96.47	8.070	87.50	15.406	64.36	22.742	16.50	30.078
99.71	1.100	96.20	8.436	86.78	15.772	62.50	23.108	14.03	30.444
99.61	1.467	95.91	8.803	86.03	16.139	60.73	23.475	11.70	30.811
99.50	1.834	95.62	9.170	85.23	16.506	58.80	23.842	9.56	31.178
99.38	2.201	95.30	9.537	84.41	16.873	56.79	24.209	7.64	31.545
99.26	2.568	94.97	9.904	83.54	17.240	54.77	24.576	5.98	31.912
99.13	2.934	94.63	10.270	82.63	17.606	52.55	24.942	4.57	32.278
99.00	3.301	94.26	10.637	81.67	17.973	50.31	25.309	3.42	32.645
98.86	3.668	93.88	11.004	80.67	18.340	48.00	25.676	2.51	33.012
98.71	4.035	93.48	11.371	79.62	18.707	45.61	26.043	1.81	33.379
98.55	4.402	93.06	11.738	78.52	19.074	43.15	26.410	1.29	33.746
98.39	4.768	92.62	12.104	77.38	19.440	40.63	26.776	0.91	34.112
98.21	5.135	92.15	12.471	76.17	19.807	38.03	27.143	0.64	34.479
98.03	5.502	91.53	12.838	74.91	20.174	35.39	27.510	0.44	34.846
97.82	5.869	91.15	13.205	73.60	20.541	32.70	27.877	0.31	35.213
97.64	6.236	90.61	13.572	72.22	20.908	29.97	28.244	0.21	35.580
97.43	6.602	90.05	13.938	70.78	21.274	27.23	28.610	0.15	35.946
97.21	6.969	89.46	14.305	69.28	21.641	24.49	28.977	0.10	36.313

---

* Refer to Figure 104; data derived using MV model with ko = 0.278 ppm/ppm-hr.. K = 15.3 ppm, Yc = 0.568 ppm/ppm, Bo = 1 ppm and So = 100 ppm!

Tabulation of 100 Randomly-Generated Numbers in the Range Between 0 and 1*

1)	0.1624	21)	0.7856	41)	0.3498	61)	0.4246	81)	0.5535
2)	0.0325	22)	0.4182	42)	0.9690	62)	0.0112	82)	0.8565
3)	0.3598	23)	0.4727	43)	0.0549	63)	0.1628	83)	0.8851
4)	0.5767	24)	0.4989	44)	0.0016	64)	0.8920	84)	0.9978
5)	0.3652	25)	0.8508	45)	0.5949	65)	0.1524	85)	0.0871
6)	0.6704	26)	0.4570	46)	0.4918	66)	0.0744	86)	0.5135
7)	0.6956	27)	0.5819	47)	0.7358	67)	0.2578	87)	0.1750
8)	0.8096	28)	0.4119	48)	0.1760	68)	0.8828	88)	0.3688
9)	0.9215	29)	0.3318	49)	0.3151	69)	0.4117	89)	0.2176
10)	0.2596	30)	0.2722	50)	0.5892	70)	0.5194	90)	0.3684
11)	0.1653	31)	0.3740	51)	0.6810	71)	0.1486	91)	0.8479
12)	0.6528	32)	0.2642	52)	0.5926	72)	0.4391	92)	0.6139
13)	0.6354	33)	0.0298	53)	0.3088	73)	0.0332	93)	0.7609
14)	0.3759	34)	0.4244	54)	0.8427	74)	0.9246	94)	0.9966
15)	0.0775	35)	0.1783	55)	0.1934	75)	0.1821	95)	0.2126
16)	0.1685	36)	0.1036	56)	0.3077	76)	0.5909	96)	0.7720
17)	0.3201	37)	0.7668	57)	0.4067	77)	0.8094	97)	0.5183
18)	0.5683	38)	0.4717	58)	0.7954	78)	0.8540	98)	0.9589
19)	0.7379	39)	0.2975	59)	0.5844	79)	0.6551	99)	0.5748
20)	0.4278	40)	0.9983	60)	0.3868	80)	0.4240	100)	0.9259

---

* As generated on the IBM PC using the Basic program "Randomize."

Tabulation of u Values for the Corresponding 100 Randomly-Generated P(u) Values from Page F-5*

1)	-0.985 u'	21)	0.790 u'	41)	-0.385 u'	61)	-0.190 u'	81)	0.135 u'
2)	-1.845 u'	22)	-0.205 u'	42)	1.865 u'	62)	-2.280 u'	82)	1.065 u'
3)	-0.360 u'	23)	-0.070 u'	43)	-1.600 u'	63)	-0.985 u'	83)	1.200 u'
4)	0.190 u'	24)	0.000 u'	44)	-2.950 u'	64)	1.240 u'	84)	2.850 u'
5)	-0.345 u'	25)	1.040 u'	45)	0.240 u'	65)	-1.025 u'	85)	-1.360 u'
6)	0.440 u'	26)	-0.110 u'	46)	-0.020 u'	66)	-1.445 u'	86)	0.035 u'
7)	0.510 u'	27)	0.205 u'	47)	0.630 u'	67)	-0.650 u'	87)	-0.935 u'
8)	0.880 u'	28)	-0.220 u'	48)	-0.930 u'	68)	1.190 u'	88)	-0.335 u'
9)	1.415 u'	29)	-0.435 u'	49)	-0.480 u'	69)	-0.225 u'	89)	-0.780 u'
10)	-0.645 u'	30)	-0.610 u'	50)	0.225 u'	70)	0.050 u'	90)	-0.335 u'
11)	-0.970 u'	31)	-0.320 u'	51)	0.470 u'	71)	-1.040 u'	91)	1.030 u'
12)	0.390 u'	32)	-0.630 u'	52)	0.235 u'	72)	-0.155 u'	92)	0.290 u'
13)	0.345 u'	33)	-1.890 u'	53)	-0.500 u'	73)	-1.835 u'	93)	0.710 u'
14)	-0.320 u'	34)	-0.190 u'	54)	1.005 u'	74)	1.440 u'	94)	2.710 u'
15)	-1.420 u'	35)	-0.920 u'	55)	-0.865 u'	75)	-0.910 u'	95)	-0.800 u'
16)	-0.960 u'	36)	-1.260 u'	56)	-0.500 u'	76)	0.230 u'	96)	0.745 u'
17)	-0.470 u'	37)	0.730 u'	57)	-0.235 u'	77)	0.880 u'	97)	0.045 u'
18)	0.170 u'	38)	-0.070 u'	58)	0.825 u'	78)	1.055 u'	98)	1.740 u'
19)	0.640 u'	39)	-0.530 u'	59)	0.210 u'	79)	0.400 u'	99)	0.190 u'
20)	-0.180 u'	40)	2.930 u'	60)	-0.285 u'	80)	-0.190 u'	100)	1.445 u'

---

* u, P(u) and u' are defined in Equation (5) on page 154!

Effect of Total Number of Data Points on Regression Results (for u' = 0)*

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior (as determined from the M2 model: $-dS/dt = 0.278\ S/(15.3 + S)$)

Experiment A: 100 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2789	15.44	0.272
2) M2	0.2786	15.42	0.279
3) MV	-0.0532	-262.37	1542
4) FV	0.000256	-	2569
5) Z2	0.1536	-	3934
6) F2	0.009811	-	4052
7) Z1	0.1778	-	4895
8) F1	0.007351	-	12582
9) ZV	0.01568	-	22911

Percent error in rate constants for M2 and M3:**

	ko	K
M2	+0.21%	+0.77%
M3	+0.32%	+0.94%

Experiment B: 34 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2788	15.43	0.284
2) M2	0.2785	15.41	0.289
3) MV	-0.0554	-270.37	1545
4) FV	0.000256	-	2509
5) Z2	0.1535	-	4182
6) F2	0.009850	-	4278
7) Z1	0.1768	-	5118
8) F1	0.007432	-	12735
9) ZV	0.01555	-	23242

Percent error in rate constants for M2 and M3:**

	ko	K
M2	+0.18%	+0.70%
M3	+0.27%	+0.83%

* No experimental error was assumed to be present.
** Percent error = ((regressed value - "real" value)/("real" value))*100%

Experiment C: 12 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2781	15.33	0.0577
2) M2	0.2781	15.33	0.0580
3) MV	-0.0642	-303.72	1484
4) FV	0.000256	-	2233
5) Z2	0.1534	-	4916
6) F2	0.009968	-	4957
7) Z1	0.1739	-	5772
8) F1	0.007672	-	13147
9) ZV	0.01515	-	23844

Percent error in rate constants for M2 and M3:

	ko	K
M2	+0.03%	+0.16%
M3	+0.05%	+0.19%

Experiment D: 10 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2780	15.31	0.0228
2) M2	0.2780	15.31	0.0229
3) MV	-0.06780	-316.76	1442
4) FV	0.000256	-	2120
5) Z2	0.1533	-	5156
6) F2	0.009998	-	5173
7) Z1	0.1730	-	5984
8) F1	0.007745	-	13242
9) ZV	0.01501	-	23926

Percent error in rate constants for M2 and M3:

	ko	K
M2	+0.01%	+0.08%
M3	+0.01%	+0.06%

Experiment E: 4 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2780	15.30	0.000440
2) M2	0.2780	15.30	0.000478
3) MV	-0.1847	-769.87	681
4) FV	0.000255	-	772
5) F2	0.0102	-	7250
6) Z2	0.1523	-	7632
7) Z1	0.1638	-	8104
8) F1	0.008406	-	13500
9) ZV	0.01347	-	22169

Percent error in rate constants for M2 and M3:

	ko	K
M2	-0.01%	-0.02%
M3	-0.02%	-0.02%

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior (as determined from the MV model: $-dS/dt = 0.278\ (1 + 0.568(100-S))S/(15.3 + S)$)

Experiment A: 100 points from 100 ppm to 0.1 ppm equally spaced with respect to time:

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2781	15.60	0.000133
2) ZV	0.2257	-	1.583
3) M3	2.979	-4.020	11.80
4) Z2	3.545	-	13.06
5) FV	0.003630	-	26.62
6) M2	1.930	-6.630	39.97
7) F2	0.2036	-	48.17
8) Z1	2.493	-	49.04
9) F1	0.1172	-	179.9

Percent error in rate constants for MV:

% error in ko = +0.04%
% error in K = +1.99%

Experiment B: 34 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2781	15.60	0.000024
2) ZV	0.2249	-	1.782
3) M3	2.998	-3.561	12.39
4) Z2	3.516	-	13.51
5) FV	0.003706	-	28.71
6) M2	1.967	-6.020	39.88
7) Z1	2.502	-	48.19
8) F2	0.2120	-	50.27
9) F1	0.1234	-	181.5

Percent error in rate constants for MV:

% error in ko = +0.03%
% error in K = +1.94%

Experiment C: 12 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2781	15.60	0.000024
2) ZV	0.2226	-	2.399
3) M3	3.009	-2.656	13.93
4) Z2	3.431	-	14.81
5) FV	0.003925	-	35.61
6) M2	2.044	-4.745	38.99
7) Z1	2.521	-	45.67
8) F2	0.2331	-	55.71
9) F1	0.1400	-	183.0

Percent error in rate constants for MV:

% error in ko = +0.04%
% error in K = +1.95%

Experiment D: 10 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2780	15.57	0.000008
2) ZV	0.2218	-	2.600
3) M3	3.013	-2.409	14.49
4) Z2	3.406	-	15.28
5) FV	0.003994	-	35.61
6) M2	2.068	-4.403	38.84
7) Z1	2.527	-	45.01
8) F2	0.2389	-	57.36
9) F1	0.1450	-	182.8

Percent error in rate constants for MV:

% error in ko = +0.002%
% error in K = +1.79%

Experiment E: 4 points from 100 ppm to 0.1 ppm equally spaced with respect to time.

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.278001	15.57	0.000002
2) ZV	0.2126	-	4.168
3) M3	1.886	-5.589	9.113
4) M2	1.549	-6.323	15.12
5) Z2	3.073	-	17.93
6) Z1	2.499	-	36.25
7) FV	0.004659	-	38.35
8) F2	0.2632	-	61.21
9) F1	0.1810	-	146.1

Percent error in rate constants for MV:

% error in ko = +0.0004%
% error in K = +1.79%

Effect of Random Experimental Error in S on Regression Results

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior modified to include random error in experimental measurements using page F-6.*

Experiment A: u' = 0.1 ppm**

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2939	17.95	169.3
2) M2	0.2891	17.52	171.2

Percent error in rate constants for M2 and M3:

	ko	K
M2	+3.99%	+14.51%
M3	+5.72%	+17.33%

Experiment B: u' = 0.25 ppm**

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2830	16.72	759.1
2) M2	0.2816	16.70	759.1

Percent error in rate constants for M2 and M3:

	ko	K
M2	+1.29%	+ 9.15%
M3	+1.80%	+ 9.28%

* 10 equally-spaced (with respect to time) S vs. t data points for the range of S from 100 ppm down to 0.1 ppm were used; variable-biomass models are inappropriate for this case and were not evaluated here.

** The other constant-biomass models are poor (performing analogously to the case in which u' = 0 on page F-8) and are not shown here.

Experiment C: u' = 0.5 ppm

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.2220	8.518	2326
2) M2	0.2368	9.521	2384
3) Z2	0.1530	-	5276
4) Z1	0.1719	-	6051
5) F2	0.01094	-	11362
6) F1	0.008025	-	22759

Percent error in rate constants for M2 and M3:

	ko	K
M2	-14.8%	-37.8%
M3	-20.2%	-44.3%

Experiment D: u' = 1.0 ppm*

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.190717	4.493952	3604
2) M2	0.208567	5.356304	3782
3) Z2	0.152568	-	5439
4) Z1	0.170667	-	6160
5) F2	0.013728	-	18951
6) F1	0.009166	-	38551

Percent error in rate constants for M2 and M3:

	ko	K
M2	-25.0%	-65.0%
M3	-31.4%	-70.6%

* Since the value of S at t = 657 hr (upon adding the correction for experimental error) was negative and use of S = 0 yields erroneous regression results for the first-order and Monod models because of the ln terms present, its value was arbitrarily assumed to be 0.01 ppm for calculations sake.

Experiment E: u' = 2.0 ppm*

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.181479	3.626129	4466
2) M2	0.198053	4.365422	4660
3) Z2	0.151813	-	5801
4) Z1	0.168296	-	6414
5) F2	0.014072	-	21941
6) F1	0.009092	-	44232

Percent error in rate constants for M2 and M3:

	ko	K
M2	-28.8%	-71.5%
M3	-34.7%	-76.3%

Experiment F: u' = 5.0 ppm*

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) M3	0.168382	2.258022	6523
2) M2	0.178733	2.650142	6632
3) Z2	0.150258	-	7143
4) Z1	0.161374	-	7441
5) F2	0.015080	-	26972
6) F1	0.009173	-	54402

Percent error in rate constants for M2 and M3:

	ko	K
M2	-35.7%	-82.7%
M3	-39.4%	-85.2%

* Since the value of S at t = 657 hr (upon adding the correction for experimental error) was negative and use of S = 0 yields erroneous regression results for the first-order and Monod models because of the ln terms present, its value was arbitrarily assumed to be 0.1 ppm for calculations sake.

Case 2: **Ideal S vs. t data from page F-4 for variable-biomass behavior modified to include random error in experimental measurements using page F-6.***

Experiment A: u' = 0.1 ppm

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2849	18.09	0.03121
2) ZV	0.2215	-	2.549
3) FV	0.003797	-	27.70

Percent error in rate constants for MV:

% error in ko = +2.48%
% error in K = +18.24%

Experiment B: u' = 0.25 ppm

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2897	20.04	0.1610
2) ZV	0.2210	-	2.534
3) FV	0.003663	-	22.64

Percent error in rate constants for MV:

% error in ko = +4.22%
% error in K = +30.95%

Experiment C: u' = 0.5 ppm

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2923	21.39	0.5758
2) ZV	0.2203	-	2.717
3) FV	0.003557	-	15.43

Percent error in rate constants for MV:

% error in ko = +5.15%
% error in K = +39.79%

* 10 equally-spaced (with respect to time) S vs. t data points for the range of S from 100 ppm down to 0.1 ppm were used; constant-biomass models are poor (performing analogously to the case in which u' = 0 on page F-11) and are not shown here.

Experiment D: u' = 1.0 ppm

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.2927	22.16	2.531
2) ZV	0.2194	-	4.349
3) FV	0.003464	-	17.82

Percent error in rate constants for MV:

% error in ko = +5.30%
% error in K = +44.85%

Experiment E: u' = 2.0 ppm

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	0.4756	72.27	28.72
2) FV	0.003496	-	34.15
3) ZV	0.2295	-	35.32

Percent error in rate constants for MV:

% error in ko = +71.07%
% error in K = +372.4%

Experiment F: u' = 5.0 ppm*

Model	ko(ppm/ppm-hr)	K(ppm)	Avg(t-tcalc)^2
1) MV	N/A	N/A	N/A
2) ZV	N/A	-	N/A
3) FV	N/A	-	N/A

* Regression results for this case are indeterminate because of negative values within ln functions (i.e., Bo + YcSo - YcS is negative for each variable-biomass model for the second point of the set, thereby making ln(Bo + YcSo-YcS) indeterminate for that point and, hence, the entire set).

Effect of Total Number of Data Points on Regression Results for Case 1 (Constant-Biomass Behavior Assumed) and u' Not equal to 0

Experiment A: u' = 1.0 ppm

	M2 Model		
Number of Points*	% Error in ko	% Error in K	Avg (t-tcalc)^2
100-4 = 96	-3.9%	-1.4%	1307
34-1 = 33	-5.2%	-2.5%	1703
12-0 = 12	+9.9%	+53.1%	1972
10-1 = 9	+87.9%	+156.0%	977
4-0 = 4	+85.4%	+321.3%	1299

Experiment B: u' = 5.0 ppm

	M2 Model		
Number of Points*	% Error in ko	% Error in K	Avg (t-tcalc)^2
100-11 = 89	-13.7%	-7.2%	4010
34-3 = 31	-12.0%	+3.1%	3525
12-1 = 11	+93.2%	+515.7%	3216
10-1 = 9	-24.6%	-37.9%	7128
4-0 = 4	-49.8%	+119.2%	11985

* Data points for which negative S values resulted, upon addition of random error terms, were excluded; this, in turn, has the effect of inflating the average S value in the latter portion of the set which otherwise would be obtained, thereby introducing a systematic error into the regression analysis results.

Effect of Data Spacing/Regularity on Regression Results*

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior modified to include random error in experimental measurements of magnitude u' = 1.0 ppm using page F-6.

S vs. t Data Points Used**	M2 Model % Error in ko	M2 Model % Error in K	M2 Model avg (t-tcalc)^2
A) 1,2,3,4,5,6,7,8,9,100	-10.4%	+ 36.2%	4.1
B) 1,91,92,93,94,96,97,98,99,100	-50.7%	-101.4%	465.5
C) 1,46,47,48,49,50,51,52,53,100	+55.3%	+247.5%	34.4
D) 1,12,23,34,45,56,67,78,88,100	-11.1%	- 19.9%	2636.3
E) 1,4,22,36,37,51,70,76,81,100	+14.0%	+ 64.5%	1533.8

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior modified to include random error in experimental measurements of magnitude u' = 1.0 ppm using page F-6.

S vs. t Data Points Used**	M2 Model % Error in ko	M2 Model % Error in K	M2 Model avg (t-tcalc)^2
A) 1,2,3,4,5,6,7,8,9,100	-150.7%	-658.1%	0.63182
B) 1,91,92,93,94,96,97,98,99,100	- 11.1%	- 33.5%	0.67192
C) 1,46,47,48,49,50,51,52,53,100	+ 7.9%	+ 73.4%	0.04231
D) 1,12,23,34,45,56,67,78,89,100	+ 2.5%	+ 18.2%	0.03121
E) 1,4,22,36,37,51,70,76,81,100	+ 18.1%	+118.6%	4.22879

* 10 S vs. t data points of various spacings with respect to time evaluated in each case.

** The numbers listed refer to the numerical sequence within each given data set that the S vs. t data points correspond to.

Effect of Data Range/Truncation on Regression Results (for u' = 1.0 ppm)

Case 1: Ideal S vs. t data from page F-3 for constant-biomass behavior modified to include the corresponding random error correction terms from page F-6.*

Experiment A: 100 ppm → 0.1 ppm (100 - 4 = 96 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.261042	14.51390	1303
2)	M2	0.267129	15.08139	1307
3)	Z2	0.156002	-	4043
4)	Z1	0.177875	-	4801
5)	F2	0.008775	-	5574
6)	F1	0.006609	-	13006

Percent error in rate constants for M2 and M3:

	ko	K
M2	-3.91%	-1.43%
M3	-6.10%	-5.14%

Experiment B: 100 ppm → 1.0 ppm (83-0 = 83 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.279558	15.70073	165
2)	M2	0.273454	15.02311	167
3)	Z2	0.176528	-	1194
4)	Z1	0.193365	-	1488
5)	F2	0.007495	-	2590
6)	F1	0.005781	-	7021

Percent error in rate constants for M2 and M3:

	ko	K
M2	-1.63%	-1.81%
M3	+0.56%	+2.62%

* All points within the given S range which result in positive values of S (upon incorporating the random error terms) are included.

Experiment C: 100 ppm → 5.0 ppm (69 - 0 = 69 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.270413	13.58608	39
2)	M2	0.264992	12.83308	40
3)	Z2	0.196391	-	269
4)	Z1	0.207140	-	345
5)	F2	0.005983	-	1459
6)	F1	0.004765	-	3684

Percent error in rate constants for M2 and M3:

	ko	K
M2	-4.68%	-16.12%
M3	-2.73%	-11.20%

Experiment D: 100 ppm → 10 ppm (61-0 = 61 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.278158	15.29156	22
2)	M2	0.267475	13.46037	24
3)	Z2	0.205794	-	116
4)	Z1	0.213314	-	144
5)	F2	0.005009	-	725
6)	F1	0.004161	-	1808

Percent error in rate constants for M2 and M3:

	ko	K
M2	-3.79%	-12.02%
M3	+0.06%	- 0.06%

Experiment E: 100 ppm → 25 ppm (47-0 = 47 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.266653	12.16970	23.4
2)	M2	0.252919	9.092224	24.6
3)	Z2	0.219454	-	33.6
4)	Z1	0.221753	-	35.1
5)	F2	0.003979	-	236.4
6)	F1	0.003479	-	546.4

Percent error in rate constants for M2 and M3:

	ko	K
M2	-9.02%	-40.57%
M3	-4.08%	-20.46%

Experiment F: 25 ppm → 0.1 ppm (54-4 = 50 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.129580	4.971184	2197
2)	M2	0.180118	7.698579	2312
3)	Z2	0.072288	-	3093
4)	F2	0.013911	-	3185
5)	Z1	0.094949	-	3771
6)	F1	0.011448	-	3897

Percent error in rate constants for M2 and M3:

	ko	K
M2	-35.2%	-47.9%
M3	-53.4%	-67.5%

Experiment G: 25 ppm → 1 ppm (37-0 = 37 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	0.253176	13.46697	339
2)	M2	0.300267	17.04119	343
3)	F2	0.012084	-	442
4)	F1	0.010882	-	546
5)	Z2	0.098019	-	633
6)	Z1	0.118861	-	844

Percent error in rate constants for M2 and M3:

	ko	K
M2	+8.01	+11.38%
M3	-8.93%	-11.98%

Case 2: Ideal S vs. t data from page F-4 for variable-biomass behavior modified to include the corresponding random error correction terms from page F-6.*

Experiment A: 100 ppm → 0.1 ppm (100-1 = 99 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	MV	0.298088	22.06903	7.1
2)	ZV	0.226277	-	8.8
3)	FV	0.003423	-	23.1

Percent error in rate constants for MV:

% error in ko = +7.23%
% error in K = +44.24%

* All points within the given S range which result in positive values of S (upon incorporating the random error terms) are included.

Experiment B: 100 ppm → 1 ppm (94-0 = 94 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	MV	0.295849	21.21199	7.4
2)	ZV	0.230337	-	8.2
3)	FV	0.003197	-	17.3

Percent error in rate constants for MV:

% error in ko = +6.44%
% error in K = +38.64%

Experiment C: 100 ppm → 5 ppm (89-0 = 89 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	MV	0.298154	21.99877	7.8
2)	ZV	0.233401	-	8.2
3)	FV	0.003004	-	13.2

Percent error in rate constants for MV:

% error in ko = +7.25%
% error in K = +43.78%

Experiment D: 100 ppm → 10 ppm (86-0 = 86 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	MV	0.318803	29.43962	8.0
2)	ZV	0.234781	-	8.4
3)	FV	0.002887	-	10.7

Percent error in rate constants for MV:

% error in ko = +14.68%
% error in K = +92.42%

Experiment E: 100 ppm → 25 ppm (80-0 = 80 points)

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	MV	0.390794	56.02126	8.6
2)	ZV	0.237064	-	8.9
3)	FV	0.002755	-	9.2

Percent error in rate constants for MV:

% error in ko = +40.57%
% error in K = +266.15%

Experiment F: 25 ppm → 0.1 ppm (21-1 = 20 points)*

	Model	ko (ppm/ppm-hr)	K (ppm)	Avg (t-tcalc)^2
1)	M3	10.43156	12.01492	0.54
2)	MV	0.267794	18.44074	0.55
3)	M2	10.58294	12.23708	0.55
4)	FV	0.009885	-	0.70
5)	F2	0.517383	-	0.81
6)	F1	0.520679	-	0.84
7)	Z2	3.379951	-	1.09
8)	Z1	4.447615	-	1.15
9)	ZV	0.090448	-	1.19

Percent error in rate constants for MV:

% error in ko = -3.67%
% error in K = +20.53%

* Bo for this case equals (1 + 0.568 (100-25)) ppm or 46.3 ppm.