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MODELING AND SIMULATION OF A SOIL-BASED MICROBIAL TREATMENT PROCESS

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Summary

A numerical model incorporating axial dispersion, first-order reversible adsorption, and several forms of a biological reaction term was developed to simulate experimental responses of microbially active soil columns. A first-order biological reaction term performs adequately after a microbial community has been developed fully. However, first-order kinetics does not adequately describe reactor responses during development of the microbial population. The applicability of Monod kinetics has also been examined. The use of a Monod-type biological reaction term adequately represented the behavior throughout bioreactor operation. In addition, organic solutes have been divided into two fractions, utilizable and non-utilizable as microbial substrate, on a percentage basis. Calibration and verification of the model was accomplished by utilizing data from three experiments.

Introduction

A soil-based microbial treatment process for on-site treatment of hazardous industrial wastewaters has been developed [1]. The indigenous microflora of the soil is supplemented by addition of an inoculum of an acclimated mixed microbial population. Wastewater, balanced with buffer and appropriate nutrients, is allowed to percolate through the soil bed. Effluent is collected, in entirety, allowing mass balances to be performed. Daily, batchwise influent additions result in cyclic reaeration and flooding. An aerobic population develops near the surface, while anaerobic organisms must dominate at greater depths. Laboratory and pilot-scale field experiments with this system have been conducted over a period of four years. An extensive data base has been collected [1—4].

Experiments have employed this biodegradation process in beds packed with soil, to oxidize organic solutes in waste liquors. Laboratory and pilot-scale bioreactor columns have been used; at both scales, vacuum has been applied at the base of vertical columns to balance capillary forces and mimic so-called "field status". The goal of these experiments is to develop design criteria for in-situ microbial treatment, immediately in or adjacent to uncontrolled dump or spill sites.

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The approach allows natural selection to control the microbial community as completely as possible. External control is achieved through management of independent parameters such as soil type, depth to groundwater, loading rates, nutrient additions, etc. A mixed microbial population is established in the soil structure. The indigenous microflora of the soil is supplemented through addition, at the soil surface, of a mixed microbial population derived from the secondary sludge of a municipal sewage treatment facility.

Microbial communities propagate through the soil column and permeate the soil structure. Leachate feed is added at the soil surface and is allowed to diffuse through the soil, where it is subsequently adsorbed and/or degraded through aerobic and anaerobic processes.

An experimental field apparatus was designed to investigate this treatment process, (1) on a scale suitable for process design, (2) under natural environmental conditions and (3) over a prolonged period of time. To fulfill these goals, a pilot-scale treatment system consisting of six soil columns, termed self-contained lysimeters (SCLs), 60 cm in diameter and 120 cm deep was built. The SCLs were designed for complete effluent recovery, implanted in the ground and operated in simulation of field conditions. Data for bioreactor modeling were obtained from Experiment 0682, started in June 1982 and lasting 161 days [1].

Parallel experiments were conducted on a laboratory scale [4, 5]. Laboratory soil columns 7.6 cm in diameter and a packing depth of 46 cm were employed. Typical duration for each experiment was 60 to 90 days. Data from these experiments were used for development and testing of the numerical model, also.

The packed bed bioreactor is a complex system that exhibits convective and dispersive flow contributions, physical adsorption and chemisorption, catalyzed non-biochemical reactions and aerobic and anaerobic mixed microbial reactor domains. With this diversity of hydraulic, physical and chemical influences, the development of a performance correlation and generalized design criteria is very difficult. Fully deterministic modeling is not possible. Thus, a step-by-step approach using incomplete models, as appropriate to limit state operations, was chosen. Ultimately, it is planned to couple these models in a comprehensive design scheme.

Experimental responses

Soil column responses are the result of three major competing processes: dispersion, adsorption and biodegradation. During operation of the microbially active soil columns, one or more of these processes may control, in different time intervals. Thus, column responses can be separated into three phases. Phase I is the period of initial operation. Microbial populations are small, and adsorption and dispersion are the processes that dominate TOC reduction. This phase closely resembles a classic adsorption breakthrough response.

Phase II is the period after the sorptive capacity of the soil has been exhausted. A decline in effluent TOC is generally observed. This results from acclimation, including natural selection, and development of the microbial population. Phase III is the period after the microbial population has developed fully. Sufficient microflora is present to degrade most, if not all, available substrate. A typical response curve is presented in Fig. 1. Phase I occurs approximately between days 1 and 37, Phase II is between days 37 and 60, and Phase III occurs after day 60.

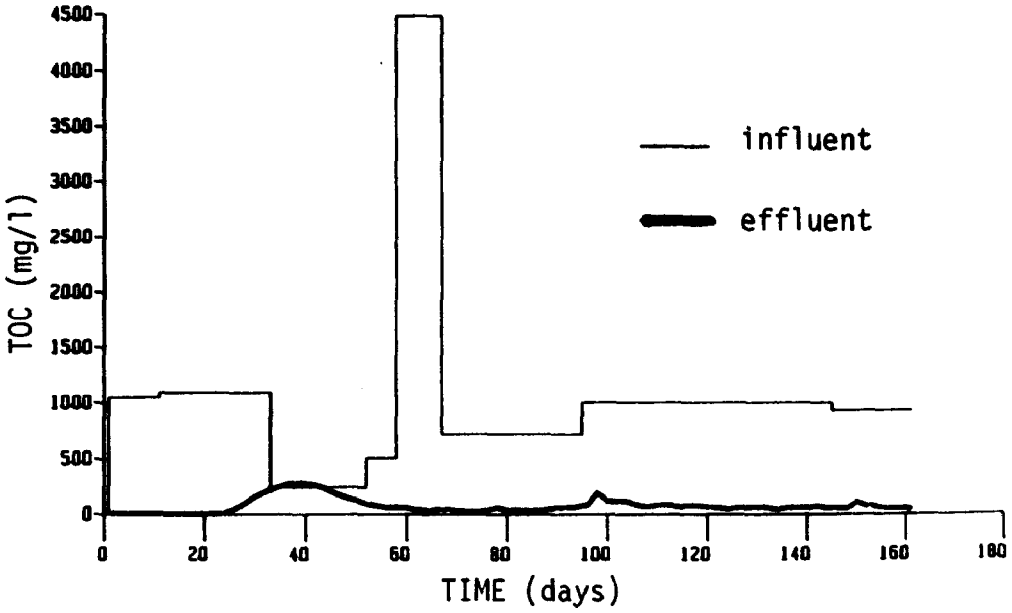

Fig. 1. Influent and effluent TOC (experimental).

Dispersion model

A dispersion model, assuming negligible radial dispersion, in conjunction with a modified F-statistic was employed by Ahlert et al. [6] to estimate packed bed porosity and longitudinal dispersion. The dispersion model is

$$\frac{\partial c}{\partial t} = E_z \left(\frac{\partial^2 c}{\partial z^2}\right) - \bar{u}_p \frac{\partial c}{\partial z} \tag{1}$$

Wen and Fan [7] demonstrated that the boundary conditions required for continuity are

$$\left(\frac{\partial c}{\partial z}\right)_{z=L} = 0 \tag{2}$$

$$\bar{u}_p c_{z\to 0^-} = \bar{u}_p c_{z\to 0^+} - E_z \left(\frac{\partial c}{\partial z}\right)_{z\to 0^+} \tag{3}$$

Estimates obtained for packed bed porosity and the dispersion coefficient, E_z, were 40.6% and 6 cm^2/day [6.5×10^{-3} ft^2/day], respectively.

Adsorption

An extension of eqn. (1) to include first-order reversible adsorption has been presented by Bear [8]

$$\frac{\partial c}{\partial t} = E_z \left(\frac{\partial^2 c}{\partial z^2}\right) - \bar{u}_p \left(\frac{\partial c}{\partial z}\right) - \left(\frac{\rho k'}{\theta_s}\right) \frac{\partial c}{\partial t} \tag{4}$$

or

$$\frac{\partial c}{\partial t} = \frac{E_z}{R_c} \left(\frac{\partial^2 c}{\partial z^2}\right) - \frac{\bar{u}_p}{R_c} \left(\frac{\partial c}{\partial z}\right) \tag{5}$$

where

$$R_c = \left(\frac{\rho k'}{\theta_s} + 1\right) \tag{6}$$

R_c is frequently referred to as a "retardation factor." Solution of eqn. (5) employing the "classic explicit" finite difference approximation described by Lapidus and Pinder [9] results in the algebraic equation

$$c_{i+1,j} = \left(\frac{2E_z h + \bar{u}_p hk}{2R_c k^2}\right) c_{i,j-1} + \left(\frac{R_c k^2 - 2E_z h}{R_c k^2}\right) c_{i,j} + \left(\frac{2E_z h - \bar{u}_p hk}{2R_c k^2}\right) c_{i,j+1} \tag{7}$$

Stability of the numerical solution is assured if

$$h < R_c k^2 / 2E_z \tag{8}$$

and

$$k < 2E_z / \bar{u}_p \tag{9}$$

Assuming adsorption and dispersion are the processes that control Phase I of the reactor operation, an estimate of R_c can be obtained. R_c was estimated to be approximately 1.2; refer to Fig. 2.

Biodegradation

Piver and Lindstrom [10] suggest that a first-order rate expression is applicable to biodegradation of landfill leachates in soil systems. Thus, eqn. (5) can be extended

$$\frac{\partial c}{\partial t} = \frac{E_z}{R_c} \frac{\partial^2 c}{\partial z^2} - \frac{\bar{u}_p}{R_c} \frac{\partial c}{\partial z} - \frac{K^*}{R_c} c \tag{10}$$

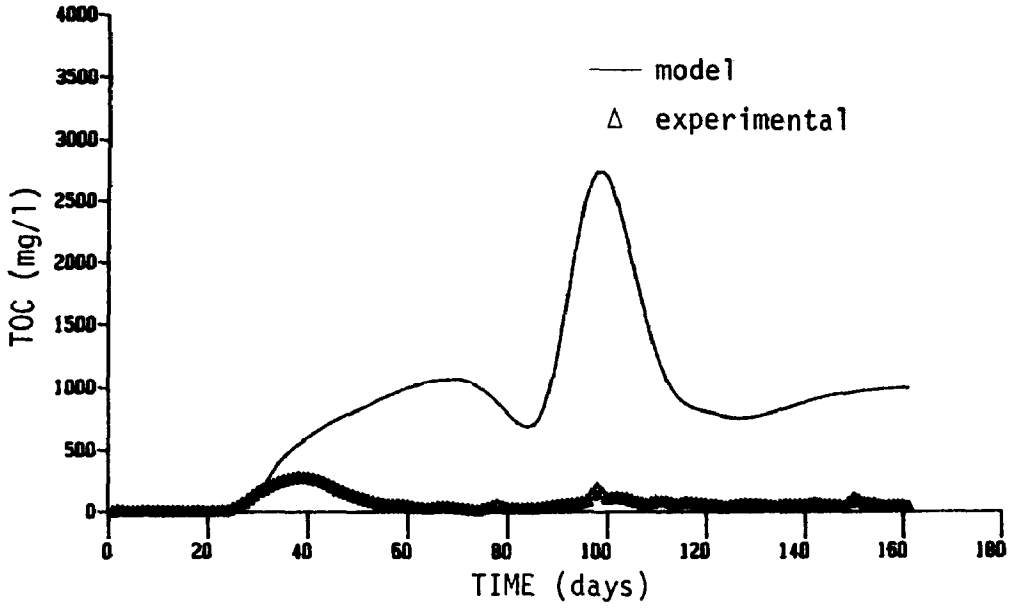

Fig. 2. Model with dispersion and adsorption, only (E_z = 6 cm²/day, R_c = 1.2).

The same finite difference methodology applied to eqn. (5) can be applied to eqn. (10). The resulting algebraic equation is

$$c_{i+1,j} = \left(\frac{2E_z h + \bar{u}_p hk}{2R_c k^2}\right) c_{i,j-1} + \left(\frac{R_c k^2 - 2E_z h - k^2 K^* h}{R_c k^2}\right) c_{i,j} + \left(\frac{2E_z h - \bar{u}_p hk}{2R_c k^2}\right) c_{i,j+1} \tag{11}$$

Stability of eqn. (11) is assured if

$$h < \frac{R_c k^2}{2E_z + k^2 K^*} \tag{12}$$

and

$$k < \frac{2E_z}{\bar{u}_p} \tag{13}$$

Sensitivity of this model to K^* is described in Fig. 3. This model simulates Phase III of soil column responses for K^* = 0.065 day^{-1}. Note, this model underpredicts effluent TOC for Phases I and II. A fully developed microbial population is assumed for the estimation of K^*. This assumption is not valid for Phases I and II.

A second approach to the biodegradation term is to assume that the

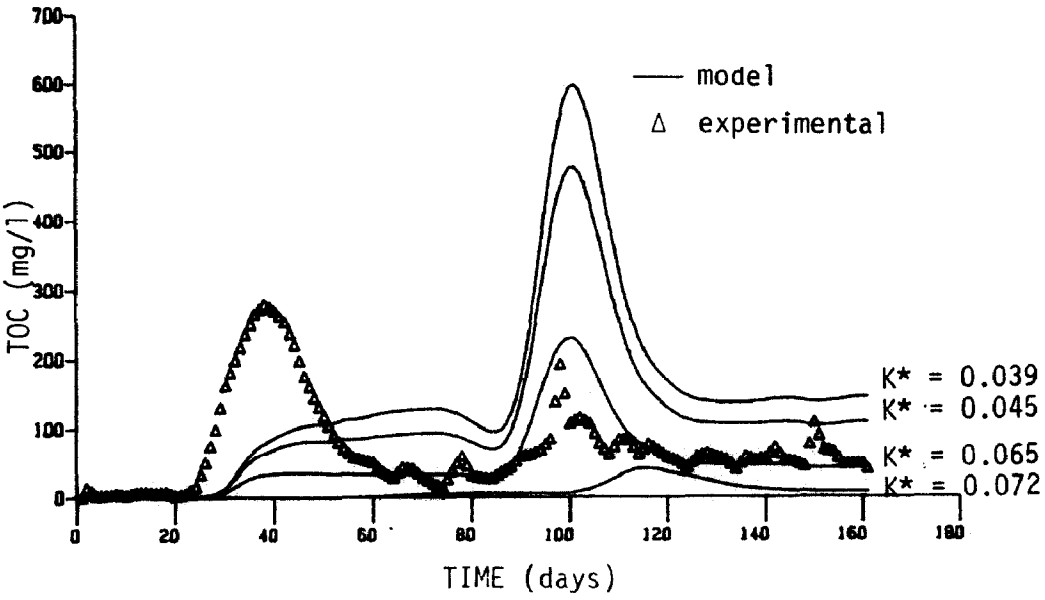

Fig. 3. Model sensitivity to $K^*(\text{day}^{-1})$ (E_z = 6.0 cm²/day, R_c = 1.2).

influent TOC is composed of a biodegradable fraction and a non-biodegradable (refractory) fraction, i.e.

$$c = A + B \tag{14}$$

where A is the non-biodegradable fraction, and B is the biodegradable fraction.

If the biodegradable and non-biodegradable fractions are assumed independent, such that

$$\frac{\partial A}{\partial B} = 0 \tag{15}$$

then

$$\frac{\partial c}{\partial t} = \frac{\partial A}{\partial t} + \frac{\partial B}{\partial t} \tag{16}$$

where

$$\frac{\partial A}{\partial t} = \frac{E_z}{R_c}\frac{\partial^2 A}{\partial z^2} - \frac{\bar{u}_p}{R_c}\frac{\partial A}{\partial z} - \frac{K_A^*}{R_c} A \tag{17}$$

$$\frac{\partial B}{\partial t} = \frac{E_z}{R_c}\frac{\partial^2 B}{\partial z^2} - \frac{\bar{u}_p}{R_c}\frac{\partial B}{\partial z} - \frac{K_A^*}{R_c} B \tag{18}$$

Because A is assumed non-biodegradable, $K_A^* = 0$. The finite difference solutions of eqns. (17) and (18) are of the same form as the solutions of eqn.

(11). If the biodegradable fraction (B) is assumed to be completely assimilated during Phase III, the theoretical maximum single pass conversion can be estimated. Sensitivity to this fractional conversion is presented in Fig. 4. Note, a 5% non-biodegradable fraction provides a good simulation of the responses observed.

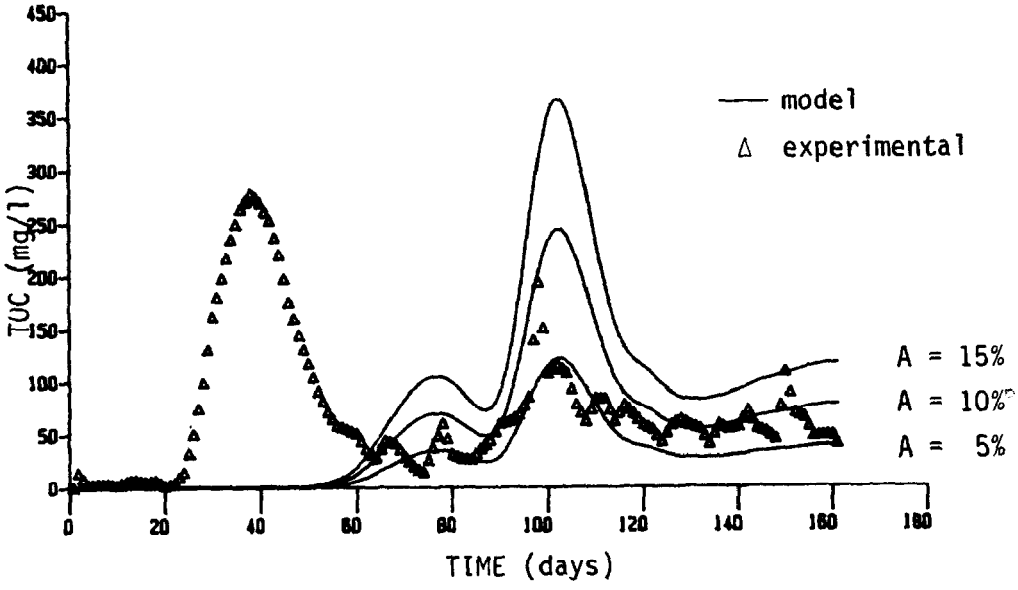

Fig. 4. Model sensitivity to non-biodegradable fraction A (E_z = 6.0 cm²/day, R_c = 1.2).

Reactor responses during microbial population development (and after development) can be simulated by the application of Monod kinetics.

The non-linear Monod reaction term incorporates cell growth with time. The rate of cell growth is given by

$$\frac{\partial x}{\partial t} = \mu x \tag{19}$$

where μ is the specific growth rate. The effect of substrate concentration, B, on growth rate is represented by

$$\mu = \frac{\mu_{max} B}{k_s + B} \tag{20}$$

Equations (19) and (20) are combined to give the following expression for cell growth rate

$$\frac{\partial x}{\partial t} = \left[\frac{\mu_{max} B}{k_s + B}\right] x \tag{21}$$

The rate of consumption of substrate is assumed proportional to the net rate of cell growth

$$\frac{\partial B}{\partial t} = -\frac{1}{y}\frac{\partial x}{\partial t} \tag{22}$$

The growth yield, y, represents the fraction of substrate converted into cell mass. Substitution of eqn. (21) into eqn. (22) yields the substrate concentration at any point in time

$$\frac{\partial B}{\partial t} = \frac{-x}{y}\left[\frac{\mu_{\max} B}{k_s + B}\right] \tag{23}$$

Initially, a high concentration of substrate exists within the bioreactor. During this time, biological development follows zero-order type kinetics. As the biodegradation (reaction) proceeds, a transition from zero-order kinetics to first-order kinetics occurs due to decreases in substrate concentration. First-order kinetics has proven effective in predicting Phase III reactor response.

Additional parameters, such as cell maintenance requirement, intracell diffusion and cell death rate, have been omitted. Thus, a lumped parameter model results. This approach necessitates the inclusion of a maximum allowable cell concentration to insure model stability. This value is the limit on microbial population density in the soil structure. An approximate value of 2000 mg/l was chosen. The model was relatively insensitive to this parameter. An upper bound for this value can be estimated based on physical density, soil porosity, etc.

The dispersion—adsorption model can be extended to include the Monod reaction term. For the biodegradable fraction of the organic solutes

$$\frac{\partial B}{\partial t} = \frac{E_z}{R_c}\frac{\partial^2 B}{\partial z^2} - \frac{\bar{u}_p}{R_c}\frac{\partial B}{\partial z} - \frac{x(t)}{yR_c}\left[\frac{\mu_{\max} B}{k_s + B}\right] \tag{24}$$

Solution of the two simultaneous differential relations, eqns. (21) and (24), can utilize the finite difference methodology described earlier. The resulting algebraic equations are

$$B_{i+j,j} = \left[\frac{2E_z h + \bar{u}_p hk}{2R_c k^2}\right] B_{i,j-1} + \left[\frac{R_c k^2 - 2E_z h}{R_c k^2}\right] B_{i,j} + \left[\frac{2E_z h - \bar{u}_p hk}{2R_c k^2}\right] C_{i,j+1} - \left[\frac{h\mu_{\max} B_{i+1,j}}{yR_c(k_s + B_{i+1,j})}\right] x_{i,j} \tag{25}$$

and

$$x_{i+1,j} = \left[\frac{h\mu_{\max} B_{i+1,j}}{k_s + B_{i+1,j}} + 1\right] x_{i,j} \tag{26}$$

TABLE 1

Feed solution compositons: Experiment 0682

Type	Dates (days)	TOC (mg/l)	GOC (mg/l)	LOC (mg/l)	Leachate vol %, No.	$(NH_4)_2SO_4$/trace elements soln. (ml/l)	1 *M* K_2HPO_4 (ml/l)
A	6/15/82–6/24/82 (01–10)	1050	1050	0	—	25	25
B	2/25/82–7/16/82 (11–32)	1100	210	890	6.6% EPA-04	5	5
C	7/17/82–8/04/82 (22–51)	230	210	20	6.6% EPA-05	5	5
D	8/05/82–8/10/82 (52–57)	510	210	300	100% EPA-05	12	6
E	8/11/82–8/19/82 (58–66)	4500	210	4290	100% EPA-05A	12	6
F	8/20/82–9/16/82 (67–94)	710	210	500	100% EPA-06	33	18
G	9/17/82–11/5/82 (95–144)	1010	210	800	4.5% EPA-07A	50	27
H	11/6/82–11/22/82 (145–161)	930	210	720	4.5% EPA-07B	50	27

$(NH_4)_2SO_4$/trace element solution contains: 50 g/l $(NH_4)_2SO_4$, 10 g/l $MgSO_4 \cdot 7H_2O$, 50 mg/l $FeCl_3 \cdot 6H_2O$, 1000 mg/l $MnSO_4 \cdot H_2O$, and 750 mg/l $CaCl_2$. All dilutions were made with dechlorinated (sparged) potable water.

Stability of the numerical solution is assured by enforcing positive concentrations. Negative concentrations are set equal to zero. A maximum allowable cell concentration, x_{max}, is defined early in the program.

The Monod model was initially tested using data from Experiment 0682 [1]. Further verification of the model was achieved by using data from Experiments 0183 and 0185 [4, 5].

Computational considerations

The finite difference equations for each model were solved using an IBM personal computer. The programs were written in BASIC and were compiled to reduce execution time. Typical time and space increments were i = 0.04 to 0.10 day and j = 0.70 to 1.1 cm. Calculated effluent TOCs were averaged over one day intervals, to mimic experimental sampling conditions. Typical execution times were 15 to 30 min, per trial case.

Experiment 0682

Experiment 0682 started in June 1982 and lasted 161 days. The experiment employed six soil columns, termed self-contained lysimeters (SCLs), 24 inches in diameter and five feet deep. Three of the SCL's were filled with a sandy loam (columns 1, 2, 3) and three with a clay loam (columns 4, 5, 6). During operation, the influent TOC consisted of eight regimes, including a dextrose feed solution for the initial development interval. The seven subsequent intervals incorporated various pretreated leachate samples. Total composition data for the feed regimes are summarized in Table 1.

Estimates of the design parameters are summarized in Table 2. The retardation factor was increased to a value of 2.6 for columns 4, 5 and 6 to represent actual reactor behavior. This was a result of the greater adsorptive capacity of the clay loam. The simulation of observed effluent TOC is shown for each of the columns in Figs. 5—10. The model predicts correctly the

TABLE 2

Design parameters of experiment 0682

Parameters	Col. No. 1	Col. No. 2	Col. No. 3	Col. No. 4	Col. No. 5	Col. No. 6
P	0.406	0.406	0.406	0.406	0.406	0.406
$F1$	1.00	1.00	1.00	1.00	1.00	1.00
$F2$	0.95	0.95	0.95	0.95	0.95	0.95
R_c	1.2	1.2	1.2	2.6	2.6	2.6
E_z	6.0	6.0	6.0	6.0	6.0	6.0
x_0	1.0	1.0	1.0	1.0	1.0	1.0
y	0.20	0.20	0.20	0.20	0.20	0.20
k_s	1500	1500	1500	1500	1500	1500
μ_{max}	1.20	2.40	1.20	0.75	0.90	1.20
x_{max}	2000	2000	2000	2000	2000	2000

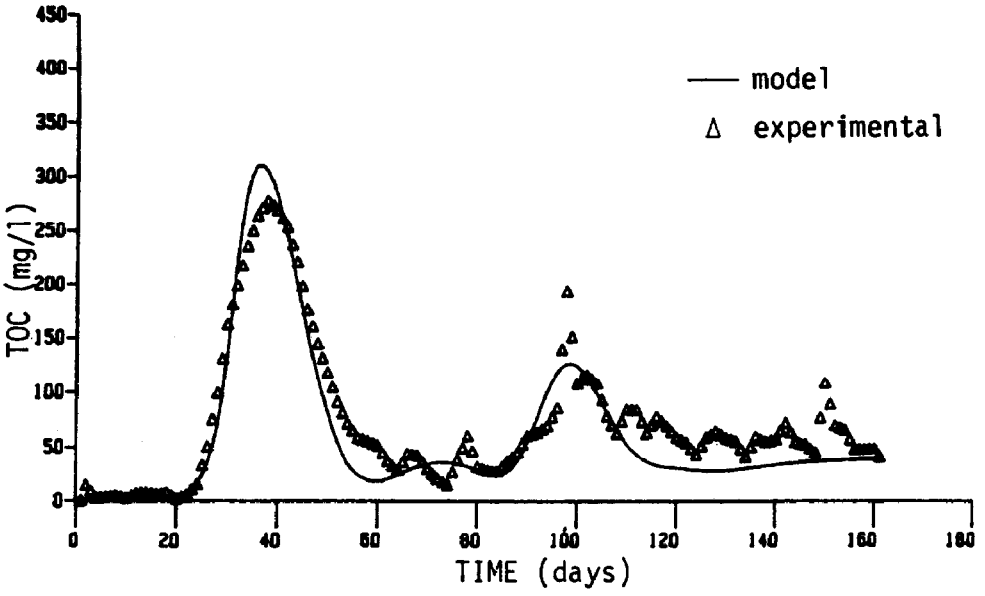

Fig. 5. Model with dispersion, adsorption and Monod kinetics (column 1).

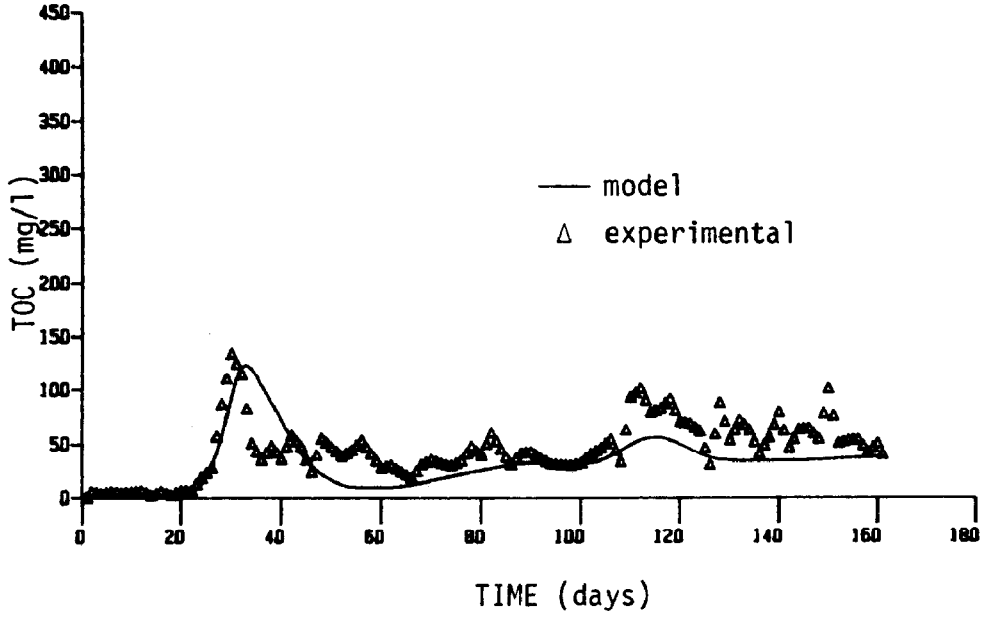

Fig. 6. Model with dispersion, adsorption and Monod kinetics (column 2).

initial phases (I and II) when the microbial community has not fully developed. A poor fit of the model is observed during phase III in Fig. 7. This was the result of channeling occurring in that particular column (SCL 3) from day 125 through day 155. Time intervals in which one or more of the competing processes is controlling are taken into account by the model.

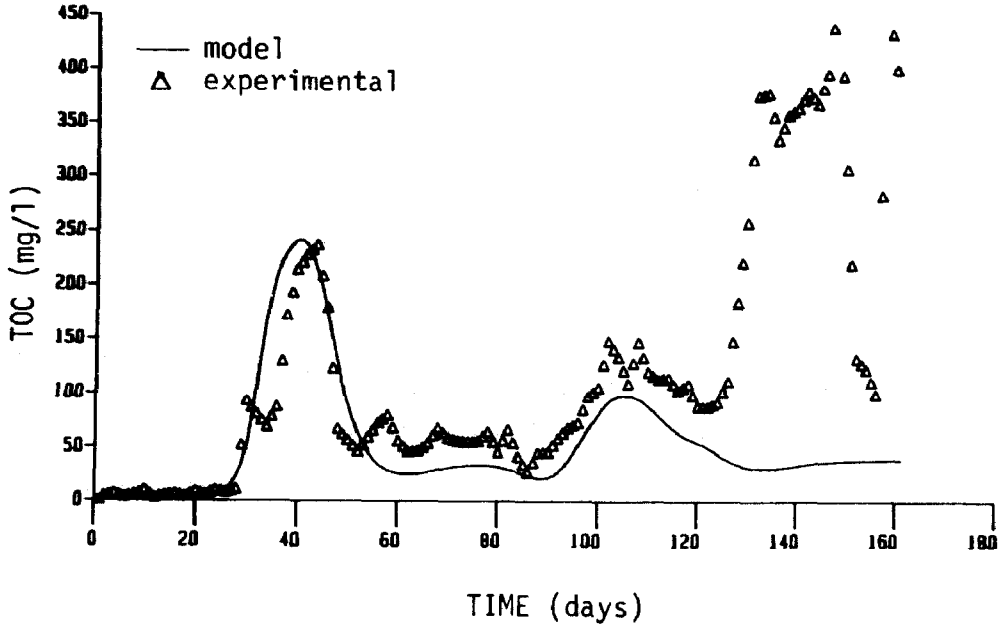

Fig. 7. Model with dispersion, adsorption and Monod kinetics (column 3).

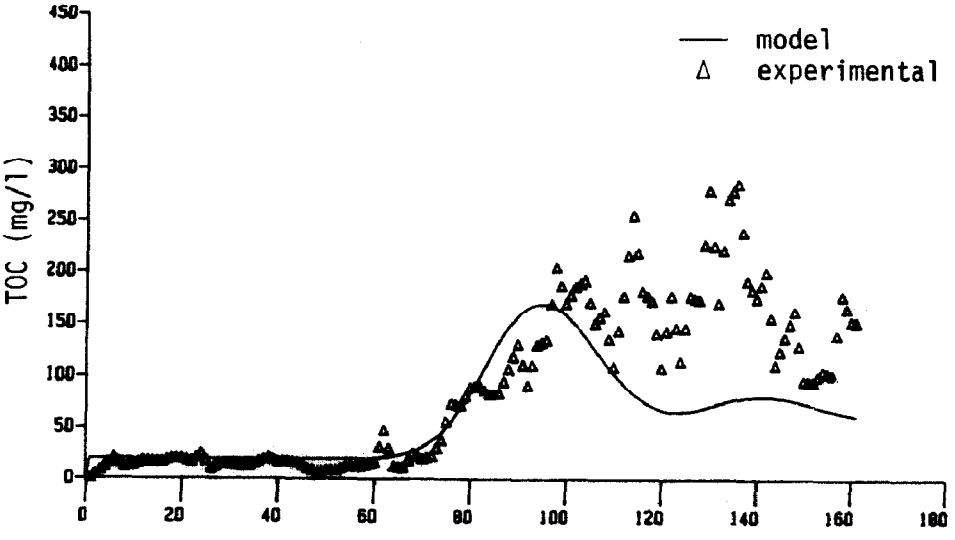

Fig. 8. Model with dispersion, adsorption and Monod kinetics (column 4).

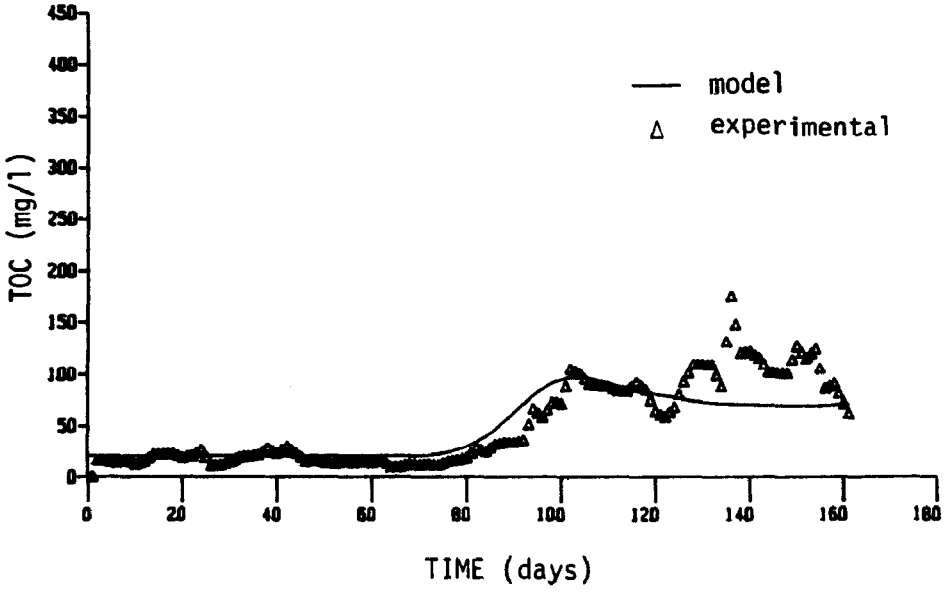

Fig. 9. Model with dispersion, adsorption and Monod kinetics (column 5).

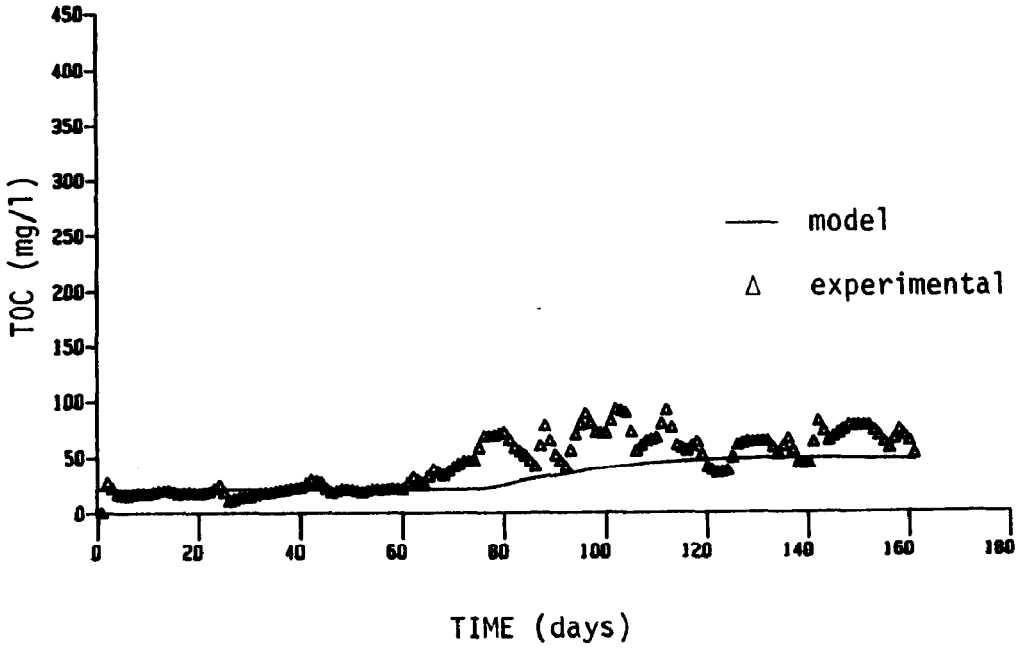

Fig. 10. Model with dispersion, adsorption and Monod kinetics (column 6).

Experiment 0183

Experiment 0183 started in January 1985 and lasted 60 days. The experiment consisted of four soil columns, three inches in diameter and 12-inches in soil depth. All four were packed with a sandy loam. On day one only, all four columns were fed influent type D, containing no leachate. Subsequent feed solutions to each column differed in leachate concentration; refer to Table 3. LC 4 served as the experimental control.

TABLE 3

Feed solution compositions: Experiment 0183

Laboratory column	Type	TOC (mg/l)	GOC	LOC	EPA-07 leachate vol %, No.	$(NH_4)_2SO_4$/trace elements soln. (ml/l)	1 *M* K_2HPO_4 (ml/l)
1	A	3000	210	2790	17.2	50	5
2	B	2000	210	1790	11.0	50	5
3	C	1000	210	790	4.0	50	5
4	D	210	210	0	0	50	5

$(NH_4)_2SO_4$/trace element solution contains: 1.0 g/l $MgSO_4$, 5.0 mg/l $FeCl_3 \cdot 6H_2O$, 100.0 mg/l $MnSO_4 \cdot H_2O$, 750.0 mg/l $CaCl_2 \cdot 2H_2O$, and 5.0 g/l $(NH_4)_2SO_4$.
Leachate properties: TOC = 16200 mg/l, TKN = 1450 mg/l, NH_3 = 1300 mg/l, total P = 14 mg/l.
Notes: (1), On day one all 4 laboratory column's fed influent Type D; (2), Each laboratory column fed particular influent type for days 2—60; and (3), All dilutions made with distilled water.

A summary of design parameters is given in Table 4. The dispersion coefficient, E_z, was determined previously to be 15 cm^2/day [6]. Figures 11, 12 and 13 compare predicted effluent concentrations with observed TOC concentrations for LC 1, LC 2 and LC 3, respectively. A steady-state microbial

TABLE 4

Design parameters of experiment 0183

Parameters	LC 1	LC 2	LC 3
P	0.406	0.406	0.406
$F1$	1.00	1.00	1.00
$F2$	0.95	0.95	0.95
R_c	1.2	1.2	1.2
E_z	15.0	15.0	15.0
x_0	1.0	1.0	1.0
y	0.20	0.20	0.20
k_s	4000	3000	1500
μ_{max}	0.60	3.0	3.0
x_{max}	2000	2000	2000

population is developed within a shorter time period as the inlet TOC concentration is decreased. The model tends to underpredict slightly the steady-state response of phase III. This must be viewed in the context of an order-of-magnitude change between influent and effluent concentrations. The model predicts an idealized response. Fluctuations of the actual data during this time could be the result of breakthrough, channeling or temperature variations within the column. A much smaller μ_{max} is observed at high influent leachate concentrations. This phenomenon has been observed independently through batch, stirred reactor experiments, also [11, 12].

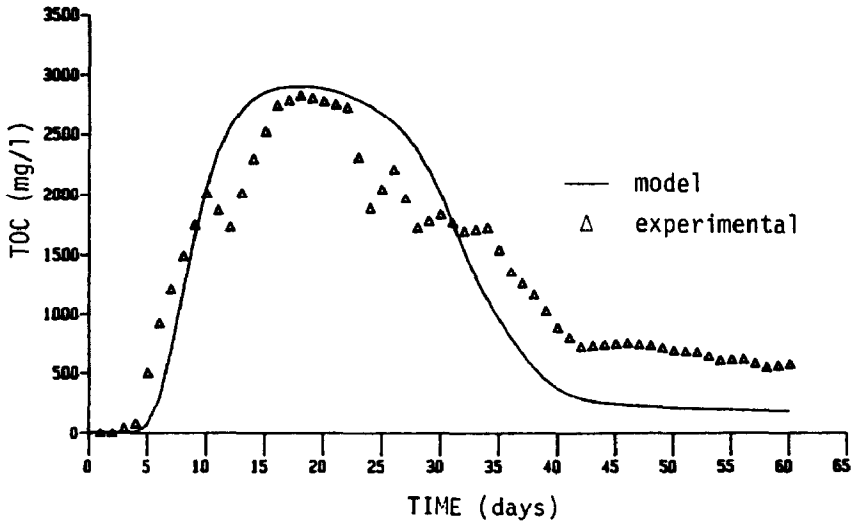

Fig. 11. Model with dispersion, adsorption and Monod kinetics (LC 1).

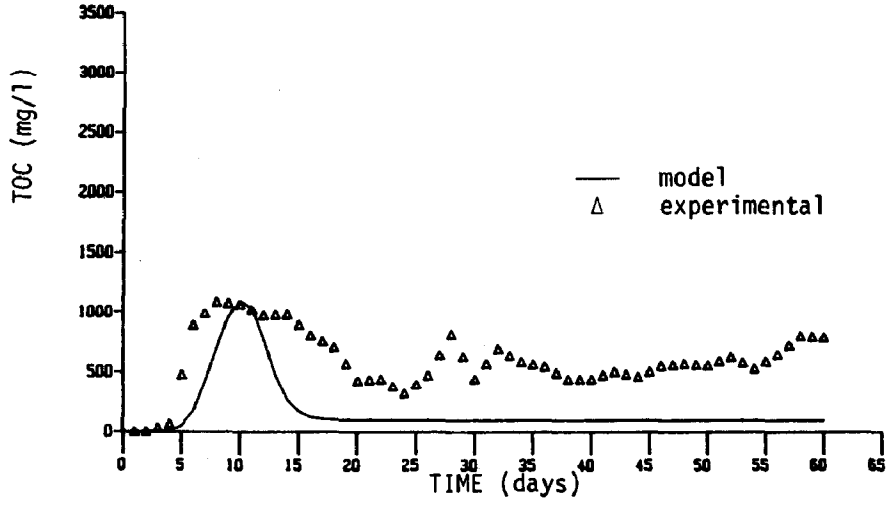

Fig. 12. Model with dispersion, adsorption and Monod kinetics (LC 2).

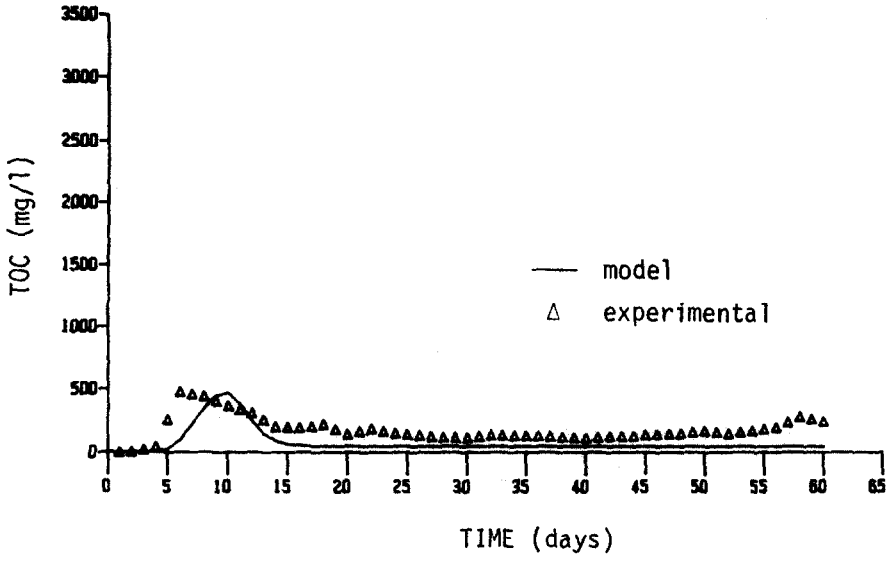

Fig. 13. Model with dispersion, adsorption and Monod kinetics (LC 3).

Sensitivity of the model to the saturation constant, k_s, is described in Fig. 14. As the saturation constant increases, the affinity of the organisms for the substrate is decreased, hence more time is required to attain a steady-state.

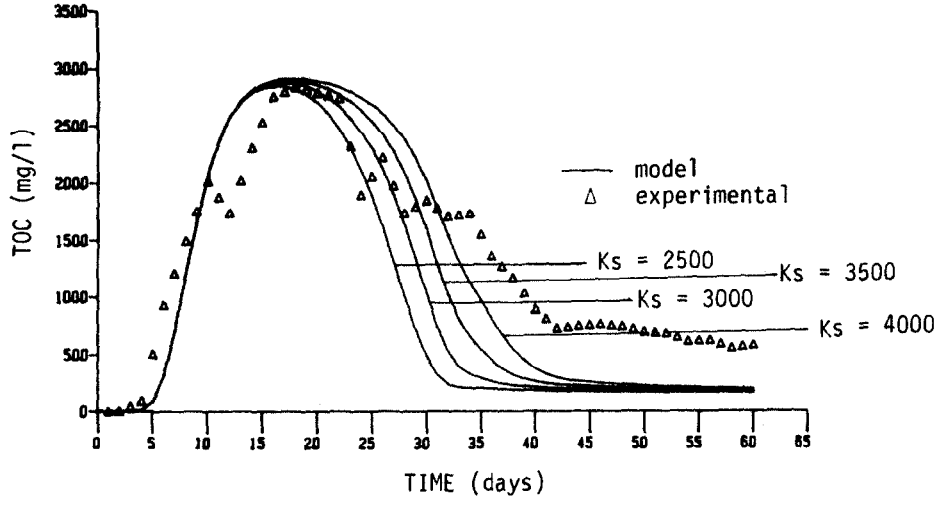

Fig. 14. Model sensitivity to k_s (mg/l) (LC 1).

Experiment 0185

Experiment 0185 started in January 1985 and lasted 60 days. The experiment employed eight laboratory columns (LCs), three inches in diameter

and 18 inches in packing depth. A 20:1 weight ratio of sandy loam soil to granular activated carbon, sieved in the sand range, was used to pack all eight columns. During the experiment, Cl^- ion was added to the influents of columns 7 and 8, as a tracer for dispersion studies. Control columns 5 and 6 were fed a solution containing 1% NaN_3 (with Ca^{2+} for three days, to inhibit microbial growth. They were used to study the effects of adsorption. Columns 3 and 4 received full strength extract (TOC = 2270 mg/l); columns 1 and 2 were fed half-strength extract (TOC = 1135 mg/l).

TABLE 5

Influent summary: Experiment 0185

Feed type	Influent TOC (mg/l)	Days fed	LCs fed	Composition (1000 ml total)
1	1135	1—57	1 and 2	400 ml secondary extract 100 ml primary extract 2.5 ml 4 *M* $Ca(NO_3)_2 \cdot 4H_2O$ 1.5 ml 0.5 *M* K_2HPO_4 496 ml distilled water
2	2270	1—57	3 and 4	800 ml secondary extract 200 ml primary extract 3.0 ml 0.5 *M* K_2HPO_4
3	2270	1—57	5 and 6	800 ml secondary extract 200 ml primary extract 10 ml 10% NaN_3 solution 5 ml 400 g Cl^-/l solution
4	0	1—7	7 and 8	5 ml 200 g Cl^-/l solution 2 ml 4 *M* $Ca(NO_3)_2 \cdot 4H_2O$/l 993 ml distilled water
SS	<1	8—14	7 and 8	5 ml 400 g Cl^-/l solution 995 ml distilled water
A	1135		1—4	25 ml 100 g glucose/l 15 ml trace element solution 15 ml 50 g $(NH_4)_2SO_4$/l 5 ml 4 *M* $Ca(NO_3)_2 \cdot 4H_2O$/l 940 ml distilled water
N	<1		5 and 6	100 ml 10% NaN_3 solution 900 ml distilled water

SAR of all feeds less than 1.4; all feeds approximately pH = 7.0; 200 g Cl^-/l solution = 414 g $CaCl_2 \cdot 2H_2O$/l distilled water; 400 g Cl^-/l solution = 500 g $CaCl_2$ + 96 g LiCl/l distilled water; 10% NaN_3 solution = 100 g NaN_3 + 362 g $Ca(NO_3)_2 \cdot 4H_2O$/l distilled water; Feeds A and N fed from 1/4/85 to 1/10/85; Feed SS fed to all LCs from 12/23/84 to 1/4/85 to achieve saturated conditions.

Feed solutions to each of the columns are shown in Table 5. It is important to note that in Experiment 0183, a different leachate source was used. In this case only, leachate was obtained through extraction of landfilled industrial sludges with dilute aqueous sodium hydroxide [13].

Table 6 summarizes relevant design parameters for Experiment 0185. Estimates for the packed bed porosity and the dispersion coefficient were 0.30 and 6.0 cm^2/day, respectively. The retardation factor was approximately 1.2. The feed solution used in Experiment 0185 was more readily biodegradable than that of Experiments 0682 and 0183. A 98% biodegradable

TABLE 6

Design parameters for experiment 0185

Design parameters	LC 1	LC 2	LC 3	LC 4	LC 5	LC 6	LC 7	LC 8
P%	30	30	30	30	30	30	30	30
$F1$	1.00	1.00	1.00	1.00	0	0	0	0
$F2$	0.98	0.98	0.98	0.98	0	0	0	0
R_c	1.2	1.2	1.2	1.2	1.2	1.2	1.0	1.0
E_z	6.0	6.0	6.0	6.0	6.0	6.0	6.0	6.0
x_0	1.0	1.0	1.0	1.0	—	—	—	—
y	0.20	0.20	0.20	0.20	—	—	—	—
k_s	1500	1500	1500	1500	—	—	—	—
μ_{max}	120.0	120.0	120.0	120.0	—	—	—	—
x_{max}	2000	2000	2000	2000	—	—	—	—

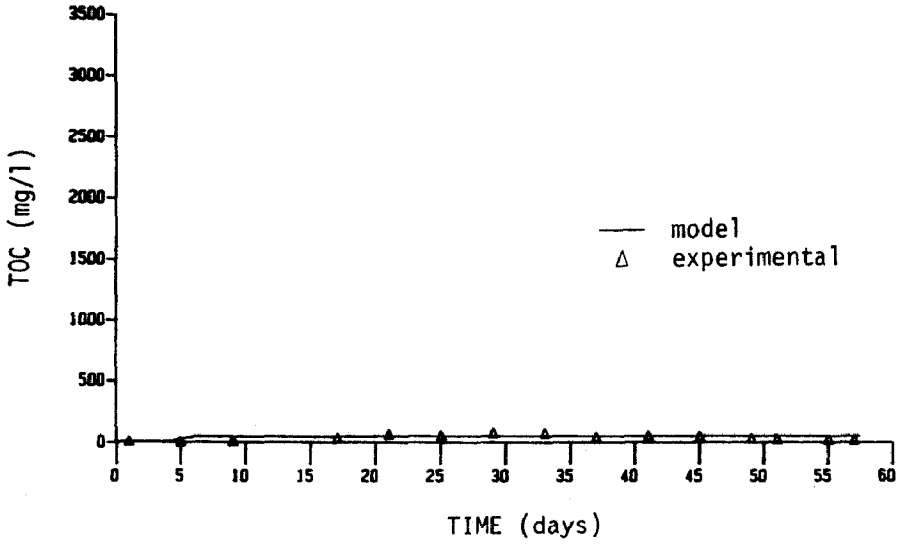

Fig. 15. Model with dispersion, adsorption and Monod kinetics (LC 3).

fraction is representative of conversion within the reactor. Figure 15 illustrates a typical comparison between predicted responses to actual responses among the column sets; LC 1 and LC 2; LC 3 and LC 4. Observed TOC responses were similar among the sets. Sensitivity to the maximum specific growth rate, μ_{max}, is described in Fig. 16. The value of μ_{max} was markedly increased to simulate the observed response. This is expected since μ_{max} is a variable parameter which depends on the characteristics of the organisms and substrate involved in the reaction. In this case, the microbial community attains a steady-state in a much shorter period of time. A μ_{max} of 120 day^{-1} provided a good prediction of the effluent data. A larger value of μ_{max} was expected, resulting from influent origin [14].

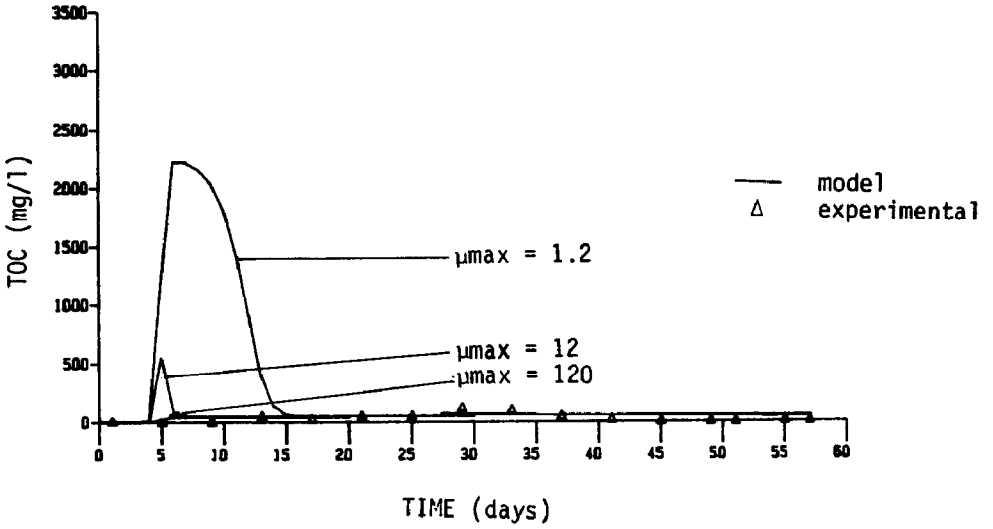

Fig. 16. Model sensitivity to μ_{max} (day^{-1}) (LC 4).

Conclusions

Several numerical models of packed bioreactors, incorporating dispersion, adsorption, and biodegradation, have been examined. First-order reversible adsorption combined with a first-order biodegradation (reaction) term provide a good simulation of microbially active soil columns after the microbial population is developed fully (Phase III). The application of Monod kinetics was adequate for prediction of observed effluent TOC concentrations throughout bioreactor operation (Phases I, II and III). Using the Monod model, design parameters were estimated for each of the columns studied. Several design parameters, i.e., k_s, and μ_{max}, fluctuated; others remained constant. Fluctuations were dependent on experimental conditions. A theoretical maximum single pass TOC reduction of 95% was estimated for Experiments 0682 and 0183. A 98% biodegradable fraction was representative of conversion within the bioreactors of Experiment 0185.

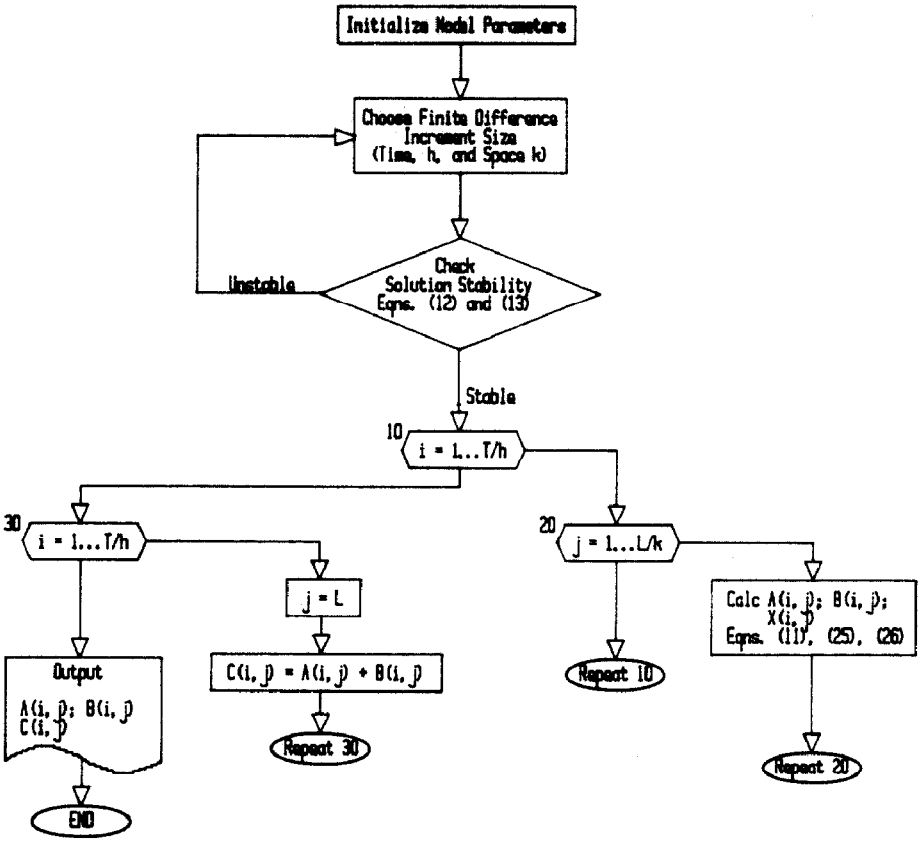

Fig. 17. Algorithm for numerical solution (not referenced in text).

List of symbols

A	non-biodegradable fraction of TOC [mg/l]
B	biodegradable fraction of TOC [mg/l]
c	TOC concentration [mg/l]
E_z	axial dispersion constant [cm^2/day]
h	time step size [day]
k	spatial step size [cm]
k'	adsorption partition coefficient [mg^{-1}]
k_s	saturation constant [mg substrate/l]
K^*	biological reaction rate constant [day^{-1}]
L	column length [cm]
R_c	retardation factor [—]
t	time [day]
$\bar{u}_p$	pore velocity [cm/day]
x_0	initial cell concentration [mg cell mass/l]
x	cell concentration at any time [mg/l]

y fraction of TOC converted to cell mass [mg cell mass/mg substrate]
z axial (vertical) distance from soil surface [cm]
ρ bulk density of dry soil [mg/l]
θ_s saturated moisture content of soil [—]
μ cell growth rate [day^{-1}]
μ_{max} maximum cell growth rate [day^{-1}]
ϕ cell loss fraction

Subscripts
i increment in time [day]
j increment in space [cm]

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