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Use of Numerical Methods in the Design of Biofilm Reactors

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ABSTRACT

Mass transfer within microbial films is described using Monod type biological kinetics in terms of the properties of packing material and the feed solution. For this purpose computer techniques have been first developed for the numerical evaluation of the normalized biofilm mathematical model. A second-order partial differential equation describing the mechanism of dispersion phenomena inside the liquid layer is then solved to determine the mass transfer coefficient. The application of the theory to experimental data reported in literature has also been demonstrated using the values of mass transfer coefficients and the computer programs developed.

Index Entries: *Biological surveys;* concentrations: design practices; diffusion; *environmental engineering;* numerical methods; *mass transfer;* mathematical models; parameters; slime; substrates; *trickling filters.*

NOMENCLATURE

A = cross-sectional area, L^2
B = dimensionless substrate concentration
B_s = dimensionless substrate concentration at the liquid-biofilm interface
$\bar{B}_{so}$ = lower limit in the definite integral $\bar{Z}$ calculated using Eq. (31)
$\bar{B}_o$ = dimensionless effluent substrate concentration corresponding to $\bar{B}_{so}$
b = total width of parallel planes in conceptual model, L
c = bulk liquid phase substrate concentration, ML^{-3}
c_o = bulk liquid phase effluent substrate concentration, ML^{-3}

c_s = substrate concentration at the liquid-biofilm interface, ML^{-3}
c_x = substrate concentration at any location x, ML^{-3}
c_i = bulk liquid phase inlet substrate concentration, ML^{-3}
C = dimensionless substrate concentration defined as c/c_i
C_x = dimensionless substrate concentration defined as c_x/c_i
D_c = diffusivity of substrate in biofilm, L^2T^{-1}
D_w = molecular diffusivity of substrate in the liquid, L^2T^{-1}
E = mass transfer coefficient defined as D_w/e, LT^{-1}
e = depth of stagnant liquid layer adjacent to biofilm, L
F = Mathematical expression to be substituted in Eq. (31) to calculate the definite integral $\overline{Z}$
H = depth of filter, L
h = liquid film thickness, L
K = dimensionless ratio of mass transfer rate to kinetic rates (*see* Eq. (B3))
K_s = Monod-half velocity coefficient, ML^{-3}
k = maximum utilization rate of rate limiting substrate, T^{-1}
k_1 = biological rate (equation) coefficient (*see* Eq. (4)), T^{-1}
k_2 = biological rate (equation) coefficient (*see* Eq. (4)), L^{-1}
k_3 = biological rate (equation) coefficient (*see* Eq. (4)), $M^{-1}\,L^3$
L = wet microbial film thickness, L
ℓ = dimensional filter length, L
M = dimensionless biofilm thickness
N = flux of substrate, $ML^{-2}\,T^{-1}$
Q_A = hydraulic loading rate, $L^3\,L^{-2}T^{-1}$
q = rate of flow per unit width, $L^3\,T^{-1}L^{-1}$
Q = volumetric rate of flow, $L^3\,T^{-1}$
S = specific surface area, $L^2\,L^{-3}$
w_{av} = average velocity of liquid in z direction, LT^{-1}
Z = dimensionless distance measured in flow direction from the origin
$\overline{Z}$ = value of the definite integral related to the filter length (*see* Eq. 31))
z = axial distance measured in flow direction from the origin, L
α = dimensionless filter depth
X = dimensionless distance measured normal to flow direction
x = dimensional distance measured normal to flow direction, L
X_c = microbial density within biofilm, ML^{-3}
γ = specific gravity, $ML^{-2}\,T^{-2}$
μ = dynamic viscosity, $ML^{-1}\,T^{-1}$
λ = effectiveness coefficient
η = biological removal ratio (biological efficiency)
η_D = $k_s h\,/\,D_w$ in which k_s is a proportionality constant in LT^{-1}

INTRODUCTION

Fixed film processes have recently received a widespread attention in wastewater technology (*14,15*). A sound understanding of kinetics of growth and substrate utilization within microbial films is essential for

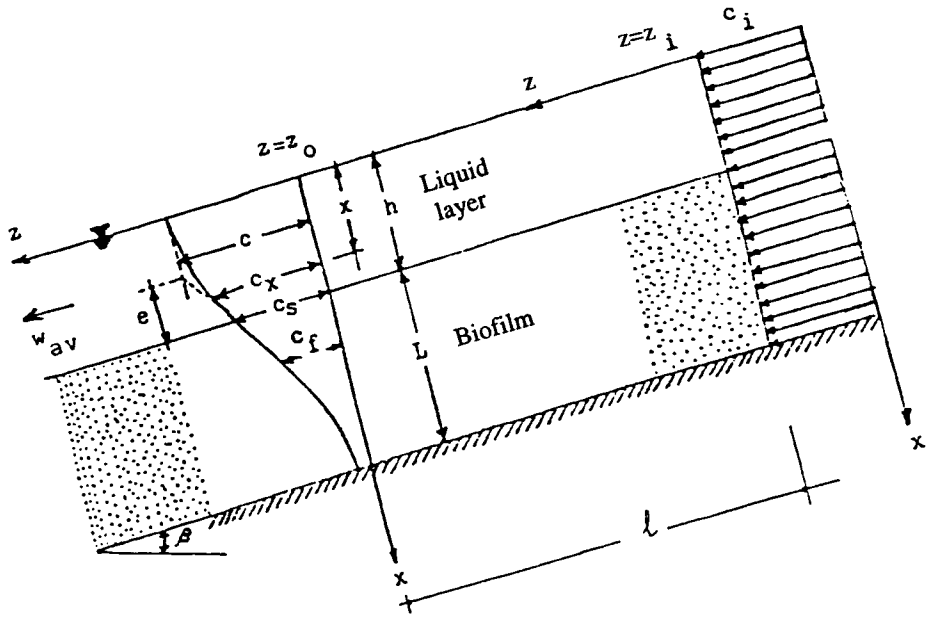

Fig. 1. Schematic of substrate distribution in inclined plane model of biofilm.

designing fixed film processes such as anaerobic filters, trickling filters, and rotating biological contactors (*2,3*). Linear and later nonlinear models using Monod-type substrate utilization rate expressions have been applied in biological filter design. The resulting equations are complicated and practically only numerical methods are left to solve such complex equation systems (*1,4*). Therefore, in this study, computer techniques were developed to evaluate the performance of biofilm reactors. The biofilm kinetic model used assumes an idealized biofilm that is characterized by a uniform density X_c, a uniform depth L, and uniform rate constants over the entire thickness of the biofilm. Substrate concentration decreases from liquid surface to biofilm surface because of the mass transfer inside the liquid layer (*8*). The flux of substrate N penetrating into the biofilm can be described according to Fick's law as

$$N = - D_w \partial c_x / \partial x \qquad \text{at } x = h \tag{1}$$

in which N = substrate flux, $ML^{-2}\,T^{-1}$; D_w = molecular diffusivity of substrate in the liquid film, L^2T^{-1}; x = length dimension normal to the biofilm surface, L; c_x = substrate concentration at any location inside the liquid layer, ML^{-3}; c_s = substrate concentration at liquid–biofilm interface, ML^{-3}; and h = liquid film depth, L (Fig. 1). However, for the sake of simplification, a bulk liquid phase substrate concentration c at an active liquid thickness, h, is combined with a stagnant liquid layer of thickness e to represent the actual concentration profile. Since no flow occurs in the stagnant liquid layer, hydrodynamic conditions remain unchanged. However, substrate is transported from the bulk liquid to the biofilm surface

through this inactive (dead) liquid layer by molecular diffusion. Therefore, the following equation can be written in place of Eq. (1) to express substrate flux N into the biofilm:

$$N \cong [D_w / e] (c - c_s) \tag{2}$$

Substrate concentration further decreases from the biofilm surface to the attachment surface as a result of the substrate utilization within the biofilm. Monod kinetic model can be used for this purpose (*16*). Within the biofilm, substrate concentration of c_f should satisfy the wall condition, $\partial c_f/\partial x = 0$ at the attachment surface. In deep biofilms, however, concentration of substrate approaches zero at this point, i.e., $c_f = 0$.

A mass balance between diffusion and reaction using Monod kinetics at any point within the biofilm leads to a differential equation that can only be solved by numerical methods in general. The most convenient solution to this equation is obtained when the mathematical problem is expressed in dimensionless terms. Atkinson and Davies (*4*) transformed the mass balance equation to the dimensionless form of:

$$(d^2f / dX^2) - M^2 f / (1 + B_s f) = 0 \tag{3}$$

using the following normalizing parameters:

$$f = c_f / c_s \; ; \; k_1 = kX_c / K_s \; ; \; M = (kX_c / D_c K_s)^{1/2} L = k_2 L \; ; \; X = x / L$$
$$k_2 = (kX_c / D_c K_s)^{1/2} \; ; \; B_s = c_s / K_s = k_3 c_s \; ; \; k_3 = 1 / K_s \tag{4}$$

in which X = dimensionless distance in x-direction; k = maximum utilization rate of rate limiting substrate, T^{-1}; K_s = Monod-half velocity coefficient, ML^{-3}; X_c = bacterial density within biofilm, ML^{-3}; D_c = the diffusivity of the substrate in the biofilm, L^2T^{-1}; M = a dimensionless microbial film thickness; f represents a dimensionless substrate concentration inside the biofilm. At the biofilm surface c_f is equal to c_s, hence, $f = 1$ when $X = 0$. At the attachment surface, however, when $X = 1$, the boundary condition becomes $df/dX = 0$ in dimensionless quantities. k_1 is a biological rate equation coefficient, T^{-1} and k_2 is a coefficient related to a solid phase diffusional limitation, L^{-1}. k_3 is also a biological rate equation coefficient, $M^{-1}L^3$.

Equation 3 was solved by Atkinson and Davies (*4*) using the Runge-Kutta-Gill method and the values of f, B_s, and df/dX were found. Substrate flux $N = -D_c(dc_f/dx)_{x=h}$ at the biofilm–liquid interface was then expressed using the dimensionless parameters defined by Eq. (4). Numerical results obtained from computer programming were plotted in form of a family of curves, whereas M and B_s changed as parameters. The following functional relationship equivalent to this family of curves was then derived by Atkinson and Davies (*4*) from the known asymptotic solution of the original mathematical problem, even though this is a semi-empirical fit of solution and may yield less exact numerical data:

$$N \cong (1 k_1 / k_2 k_3) (M B_s) / (1 + B_s) \tag{5}$$

in which λ is expressed in terms of hyperbolic functions (*see* Appendix A). For all L, but for large values of c_s, Eq. (5) is approximated by k_1L/k_3 as an asymptotic condition.

MASS TRANSFER COEFFICIENTS *E* FOR THE ASYMPTOTIC CONDITIONS

N has a number of asymptotic forms as follows:
(i) For small biofilm thickness L and for all c_s

$$\lambda \cong 1\,;\, N \cong (k_1 L c_s) / (1 + k_3 c_s) \tag{6}$$

For small c_s, however, it becomes:

$$N \cong k_1 L c_s$$
$$N \cong k_s c_s \tag{7a}$$
$$k_s = k_1 L \tag{7b}$$

in which k_s is a proportionality factor.
(ii) For large L

$$\lambda \cong (1+2k_3c_s)^{1/2} / M = (1+2k_3c_s)^{1/2} / k_2 L \tag{8}$$

For small c_s, however, it becomes $\lambda \cong (1/M)$ and substitution of this value into Eq. (5) leads to:

$$N \cong (1 / k_2 L)\,(k_1 L\, c_s) / (1 + k_3 c_s) \cong (k_1 / k_2)\, c_s = k_s c_s \tag{9}$$

in which

$$k_s = k_1 / k_2 \tag{10}$$

Inserting Eq. (7a) into Eq. (2) yields:

$$N \cong k_s c_s = (D_w / e)\,(c - c_s) \tag{11}$$

$$e = (D_w / k_s)\,(c - c_s) / c_s \tag{12}$$

Dividing both sides by h it results in

$$e / h = (D_w / k_s h)\,(c - c_s) / c_s = [1 / (k_s h / D_w)]\,(c - c_s) / c_s = (1 / \eta_D)\,(c - c_s) \tag{13}$$

in which

$$\eta_D = k_s h / D_w \tag{14}$$

If c and c_s are known, the value of (e/h) can be determined using Eq. (13) as a function of the parameter η_D. The mass transfer coefficient E hence becomes:

$$E = D_w / e = D_w / [(h)\,(e/h)] = (D_w\, \eta_D / h)\,[c_s / (c - c_s)] \tag{15}$$

If the dimensionless ratio Ek_2/k_1 is denoted with K, Eq. (15) can also be written as

$$E = D_w / e = K k_1 / k_2 = K k_1 L / k_2 L \tag{16}$$

In order to determine E, the values of c and c_s are needed. Hence, the axial dispersion inside the liquid layer should be investigated for this purpose. The liquid layer is assumed to be void of microorganisms. At the inlet section there is a uniform substrate concentration c_i. Owing to the molecular diffusion and the existence of a velocity gradient, an axial dispersion phenomenon takes place (Fig. 1). Derivation of the following dispersion equation can be found in any standard text:

$$D_w(\partial^2 c_x / \partial x^2) - [\gamma \sin\beta / 2\mu] (h^2 - x^2) (\partial c_x / \partial z) = 0 \tag{17}$$

in which β = the angle of inclined plane with the horizon; γ = specific gravity ($ML^{-2} T^{-2}$); μ = dynamic viscosity ($ML^{-1} T^{-1}$); z-axis is on the liquid surface and parallel to the flow direction whereas x-axis is normal to it. The following boundary conditions can be written:

$$\text{(i) For } x = O\,, \; - D_w \partial c_x / \partial x = O \tag{18a}$$

$$\text{(ii) For } x = h\,, \; -D_w \partial c_x / \partial x = N \tag{18b}$$

(iii) Substrate concentration c_x decreases both in z- and in x-direction and ultimately vanishes at the infinity, i.e.,

$$\text{For } z = z_i \;\; ; x \leq h \; ; \; c_x = c_i \tag{18c}$$

$$z = \infty \;\; , x \leq h \; ; \; c_x = O \tag{18d}$$

The solution of Eq. (17) becomes easier for the asymptotic condition explained earlier, namely as

$$-D_w \partial c_x / \partial x = N = k_s c_s \tag{18e}$$

and the determination of E is simplified as explained below:

SOLUTION TO DISPERSION EQUATION INSIDE THE LIQUID LAYER

Equation (17) resulting from a mass balance inside the liquid layer was solved for the special case of low concentration asymptotes $N = k_s c_s$. The following substitutions were made to normalize Eq. (17):

$$X = x / h \; ; \; Z_D = D_w z / h^2 w_{max} \; ; \; C_x = c_x / c_i \; ; \; C_s = c_s / c_i \tag{19}$$

in which w_{max} is the maximum value of the velocity w at the liquid surface. A parabolic velocity profile was assumed for newtonian fluid with

no shear or surface tension at surface (*7,12*). Equation (17) was then transformed into the following dimensionless form

$$(1 - X^2)\,\partial C_X / \partial Z_D = \partial^2 C_X / \partial X^2 \tag{20}$$

The normalized differential equation was then solved using computer techniques and the method of finite differences between $Z_D = (Z_D)_i = 0$ (or $z = z_i = 0$) and $Z_D = Z_D$ (or $z = z$). The boundary conditions expressed by Eqs. (18) now become:

$$\text{(i) For } X = 0\,,\ \partial C_x / \partial X = 0 \tag{20a}$$

$$\text{(ii) For } X = 1\,,\ \partial C_x / \partial X = -\,(k_s / D_w)\,h\,C_s = -\,\eta_D\,C_s \tag{20b}$$

$$\text{(iii) For } (Z_D) = (Z_D)_i\,,\ X < 1\,,\ C_x = 1 \tag{20c}$$

$$\text{For } (Z_D) = \infty\,,\ X < 1\,,\ C_x = 0 \tag{20d}$$

C_x was then obtained in a general way as a function of Z_D and X for different values of η_D. The value of C_x for $X = 1$ at any section of Z_D gives the required C_s value at the liquid–biofilm interface. The bulk liquid phase substrate concentration C was then calculated from the substrate flux per unit width in the main flow direction as

$$\int_0^h c_x w\,dx = c\,w_{av} h \tag{21}$$

in which w_{av} is the mean velocity of the laminar film flow over the inclined plane (LT^{-1}). Using dimensionless quantities and the parabolic velocity distribution it becomes:

$$C = c / c_i = (3/2) \int_{X=0}^{X=1} C_X (1 - X^2)\,dX \tag{22}$$

After feeding Eq. (22) into the computer program developed for the numerical solution of Eq. (20), the bulk substrate concentration C was also obtained together with the unknown concentration C_x and C_s (an example was given in Fig. 2 for $\eta_D = 5$). Using the calculated values of C_s and C, the ratio of e/h was then obtained from Eq. (13) as

$$e / h = (1 / \eta_D)\,[(c / c_i) - (c_s / c_i)] / (c_s / c_i) = (1 / \eta_D)\,(C - C_s) / C_s \tag{23}$$

They are given in Fig. 3 for different values of η_D.

The dimensionless length Z_D can be found using the physical parameters related to the filter. The value of $Z_D = (Z_D)_o$ for the outlet section is thus obtained substituting the filter depth $z = \ell$ into Eq. (19) as

$$Z_D = (Z_D)_o = D_w \ell / h^2 w_{max} = D_w \ell / [(h^2)\,(3/2)\,(w_{av})] = (2/3)\,(D_w / h)\,(\ell / q) \tag{24}$$

in which q = rate of flow per unit width of the biofilm, $L^3T^{-1}L^{-1}$. The mean velocity w_{av} can be calculated as (2/3) (w_{max}) for the parabolic velocity distribution of laminar film flow.

The conceptual model used in this study can be described by considering a filter element with a cross sectional area A and a depth H (Fig. 4).

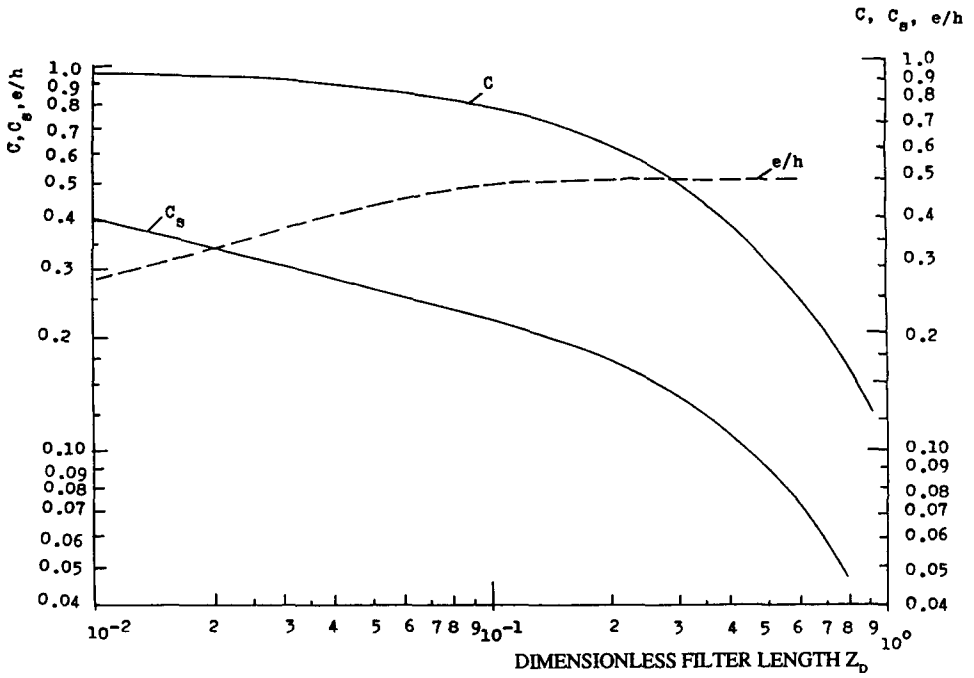

Fig. 2. Dimensionless substrate concentration C and C_s and values of e/h for different values of Z_D when $\eta_D = 5$.

If the specific surface area is S, then the surface area of the filter medium is given by $(S)(AH)$, which should be equal to the wetted area in the conceptual model, namely as,

$$bH = (SA)(H) \tag{25}$$

where b denotes the wetted perimeter. Hence

$$b = SA \tag{26}$$

This equation converts the filter media into a series of parallel planes with an angle of $\beta = \pi/2$ (namely vertical planes) of which total width is equal to $b = \Sigma b'$ where b' is the width of each parallel plane (Fig. 4). The flow rate per unit width hence becomes

$$q = C/b = Q/SA = (Q/A)/S = Q_A/S \tag{27}$$

in which Q is the volumetric flow rate passing through a filter cross-sectional area A in L^3T^{-1} and Q_A is the hydraulic loading rate in LT^{-1}.

In this section a numerical solution of Eq. (17) was given for the asymptotic forms of the substrate flux N. Its general form, however, was considered below for a steady state assumption with no axial dispersion which can be justified because of low liquid applications in many practical problems. The mathematical difficulties arising from dispersed flow was thus eliminated.

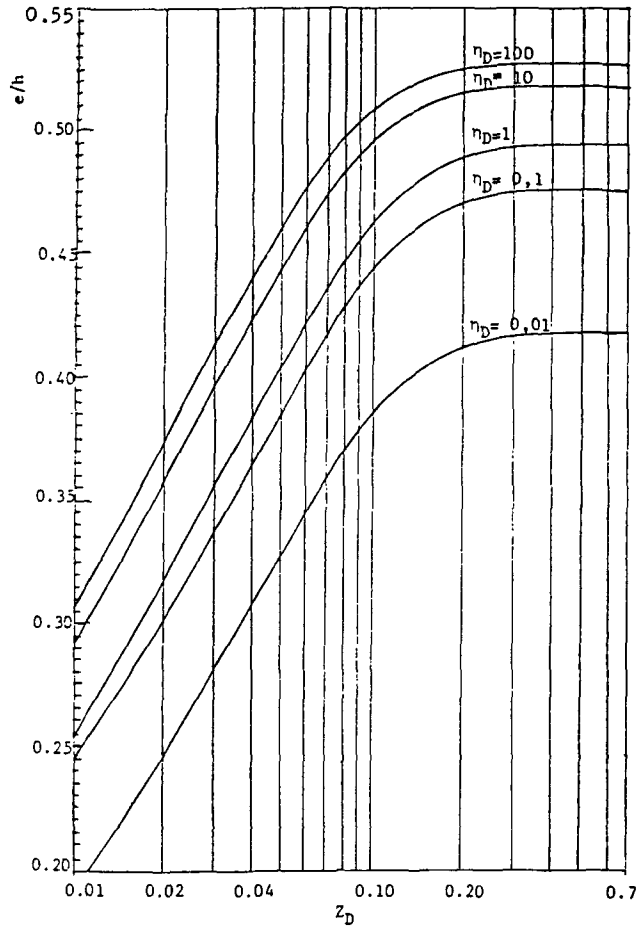

Fig. 3. Variation of the values of e/h with Z_D and η_D.

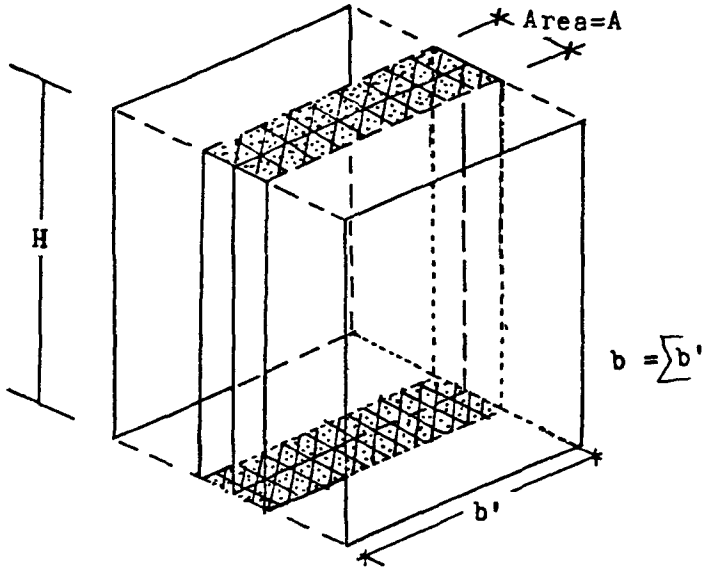

Fig. 4. Conceptual model to study biological filtration.

A BIOFILM MATHEMATICAL MODEL FOR THE GENERAL EXPRESSION OF THE SUBSTRATE FLUX *N*

A biofilm mathematical model is described below for a plug flow reactor with no concentration gradient in the x-direction. When the flow moves axially in the z-direction along the reactor, with convection being the only mode of pollutant transport, the organic constituents diffuse into the biofilm and are subsequently used (Fig. 1). A differential substrate material balance on this reactor yields:

$$q\,dc / dz = -N \tag{28}$$

The bulk liquid phase substrate concentration decreases from its initial value c_i at $z=z_i$ to a value of c at a location of $z=z_o$. These boundary conditions needed to solve Eq. (28) define the concentrations of substrate at any location along the plug flow reactor. Substituting Eq. (28) into Eq. (2) and writing the definition of E in Eq. (15) leads to

$$-q\,dc / dz = N = (D_w / e)(c - c_s) = E(c - c_s) \tag{29}$$

Equation (29) was written in terms of dimensionless parameters using Eqs. (4) and (5). Dimensionless distance in z-direction was now defined as

$$Z = k_1 z / k_2 q \tag{30}$$

Thus, dimensionless filter length $\overline{Z}$ in which dimensionless substrate concentration is reduced from any initial value of B_{si} (or B_i) to a predetermined outlet concentration of $\overline{B}_{so}$ (or $\overline{B}_o$) is obtained from

$$\overline{Z} = \int_{B_{so}}^{B_{si}} F dB_s \tag{31}$$

in which F is a function of B_s when M, L, and the other kinetic and hydraulic parameters are given (*see* Appendix B for the derivation of Eq. [31]). F is calculated using the quantities λ, g, and ϕ defined in Appendix A and B (an example is given in Table 1). For performing the numerical ingration expressed by Eq. (31), a computer program was developed (*see* Fig. 5 for the flow diagram). Table 1 gives the computer output as an example. In this example, λ, B, g, F, and $\overline{Z}$ were calculated as a function of B_s for the following data which corresponds to the experiments conducted by Atkinson and How (*5*):

$k_1 = 0.291\ s^{-1}$; $k_2 = 205.43\ cm^{-1}$; $k_3 = (1.180)(10^5)cm^3\ g^{-1}$
$D_w = (6.9)(10^{-6})cm^2\ s^{-1}$; $L = (6.5)(10^{-3})cm$; $q = (4.77)(10^{-2})cm^3 s^{-1} cm^{-1}$
$E = (3.507)(10^{-4})cm\ s^{-1}$; $\ell = 223.5cm$

The computer inputs M, K, α, A_o and A_1 were then obtained from the given data. A_o and A_1 were defined as:

$$A_o = (k_2 / k_1) q\ ;\ A_1 = 10^{-6} k_3 \tag{32}$$

Table 1
Calculation of Numerical Integral $\overline{Z}$
Between the Boundaries of $B_{so}=0.0025$ and any Value of B_{si} Using Eq. (31)

1	2	3	4	5	6	7	8	9	10
$M=1.335$; K=0.2480; $A_o=33.6734$ cm; $A_1=0.118$ cm^{3}g^{-1}; $\alpha=6.6374$; Step=0.0025									
B_s	λ	g	B	F	dZ	Z	z	mg ℓ^{-L}	η
0.0025	0.65321	0.00217	0.0113	2070.4851	0.0000	0.0000	0.00	0.095	—
0.0050	0.65438	0.00435	0.0225	1034.8281	3.8816	3.8816	130.71	0.191	—
0.0075	0.65554	0.00651	0.0338	689.6056	2.1555	6.0372	203.29	0.286	—
0.0100	0.65670	0.00868	0.0450	516.9917	1.5082	7.5454	254.08	0.381	0.691
0.0125	0.65786	0.01084	0.0562	413.4213	1.1630	8.7084	293.24	0.476	0.693
0.0150	0.65901	0.01300	0.0674	344.3727	0.9472	9.6557	325.14	0.571	0.703
0.0175	0.66016	0.01516	0.0786	295.0510	0.7993	10.4550	352.05	0.666	0.716
0.0200	0.66130	0.01731	0.0898	258.0586	0.6914	11.1464	375.34	0.761	0.713
0.0225	0.66244	0.01946	0.1010	229.2857	0.6092	11.7555	395.85	0.856	0.713
0.0250	0.66357	0.02161	0.1121	206.2665	0.5444	12.3000	414.18	0.950	0.716
0.0275	0.66470	0.02375	0.1233	187.4319	0.4921	12.7921	430.75	1.045	0.719
0.0300	0.66582	0.02589	0.1344	171.7358	0.4490	13.2411	445.87	1.139	0.717
0.0325	0.66694	0.02803	0.1455	158.4538	0.4127	13.6538	459.77	1.233	0.718
0.0350	0.66806	0.03016	0.1566	147.0688	0.3819	14.0357	472.63	1.327	0.720
0.0375	0.66917	0.03229	0.1677	137.2013	0.3553	14.3910	484.59	1.421	0.720
0.0400	0.67028	0.03442	0.1788	128.5667	0.3322	14.7232	495.78	1.515	0.719
0.0425	0.67138	0.03654	0.1898	120.9477	0.3119	15.0351	506.28	1.609	0.720
0.0450	0.67248	0.03866	0.2009	114.1748	0.2939	15.3290	516.18	1.702	0.721

(*see* Appendix B). The resulting input parameters were written in the heading of Table 1 as

$$M = 1.335\,;\, K = 0.2480\,;\, \alpha = 6.6374$$

$$A_o = (k_2 / k_1)\, q = 33.6734\,\text{cm}\,;\, A_1 = 10^{-6} k_3 = 0.118\,\text{cm}^3\, g^{-1}$$

The computer output depends upon the interval of $\triangle B_s$ selected. Table 1 was calculated using an interval of $\triangle B_s = B_{so} = 0.0025$. The values of $\overline{Z}$ in Table 1 denote the dimensionless filter lengths in which any value of inlet concentration B_{si} is reduced to $\overline{B}_{so} = 0.0025$ at the outlet. For a filter with a depth of $z=\ell$, the dimensionless filter length α is calculated using Eq. (30) as explained below. The value of α between any two outlet and inlet concentrations of B_{so} (or B_o) and B_{si} (or B_i) is equal to the difference of the corresponding $\overline{Z}$ values in Table 1 as

$$\alpha = \overline{Z}_i - \overline{Z}_o = (k_1 / k_2 q)\,(z_o - z_i) = k_1 \ell / k_2 q \tag{33}$$

On the contrary, if α is known, filter depth ℓ can be found from

$$\ell = (k_2 / k_1)\, q\, \alpha = A_o\, \alpha \tag{34}$$

The biological efficiency η corresponding to a given inlet concentration B_{si} (or B_i) then becomes:

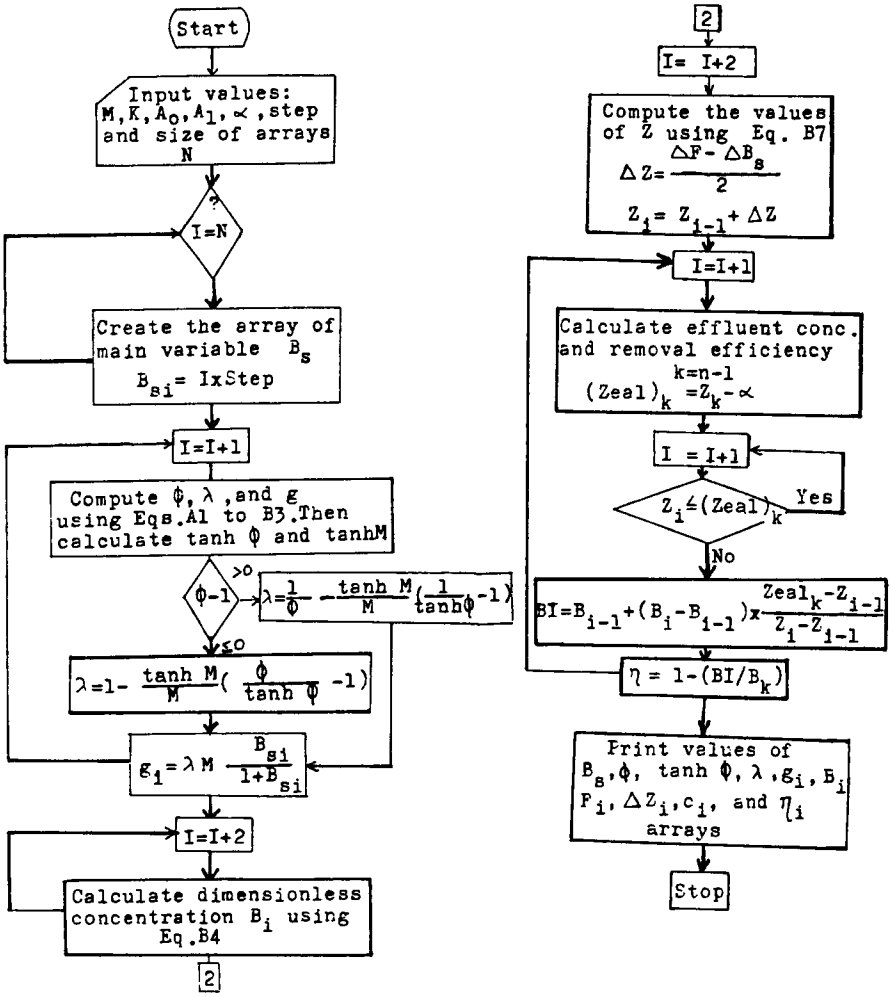

Fig. 5. Flow diagram of the computer program for the numerical integral $\bar{Z}$ between the boundaries of B_{so} and B_s.

$$\eta = 1 - 1\,(c_o / c_i) = 1 - (c_o k_3 / c_i k_3) = 1 - (B_o / B_i) \qquad (35)$$

(*see* illustrative example in Appendix C).

The calculation of biological efficiency η for different inlet concentrations B_i was also included in the computer program developed. The effect of ΔB_s on η was also investigated (*see* Appendix C). It has been found that η values change not more than 0.1% for an interval of $\Delta B_s < 0.001$. Therefore, the computer calculations were performed using a value of $\Delta B_s = 0.001$ in this study (*8,9,13*).

EVALUATION OF BIOLOGICAL PARAMETERS USING LOW AND HIGH CONCENTRATION ASYMPTOTES

The most satisfactory method of determining biological parameters k_1, k_2, and k_3 is to use the asymptotic expressions together with the experimental data obtained from a flat-plate biological film reactor because the hydraulic conditions are clear and the physical parameters can easily be defined. When c_i tends to zero, Eq. (31) reduces to (*3,6,14*):

$$\ln (c_o / c_i) \cong - [K \tanh M / (K + \tanh M)] \alpha \tag{36}$$

For thin biofilms ($M < 0.5$), when $c_i \rightarrow 0$, Eq. (36) becomes:

$$\ln (c_o / c_i) \cong - K\alpha / [(K/M) + 1] \tag{37}$$

On the other hand, for all values of L, when c_i is sufficiently large, Eq. (31) reduces to

$$\eta = 1 - (c_o / c_i) \cong (k_1 L / k_3) (\ell / q) (1 / c_i) = (I) (1 / c_i) \tag{38}$$

in which

$$I = (k_1 L / k_3) (\ell / q) \tag{39}$$

(*see* Appendix B for its derivation). If the experimental data are accordingly replotted in terms of η versus $(1/c_i)$, the result is a linear relationship at high concentrations with a slope of I. Applications of these equations to obtain the biological system parameters from the experimental data will be explained below.

EXPERIMENTAL CONFIRMATION

In order to check the computer programs developed, the experimental results published by Atkinson and How (*5*) were evaluated. Three different series of experiments were conducted. In the first experiment, the feed solution made up glucose was used to develop a microbial film on a glass plate (thin biofilm). The length of the biofilm was $\ell = 223.5$ cm, the width of the biofilm was $b = 18.5$ cm, and the rate of flow was $Q' = 53$ cm^3 min^{-1}. The measured values of the biological efficiencies η were plotted in Fig. 6 against the inlet glucose concentration c_i.

In these experiments, velocity measured on the liquid surface was $w_{max} = 1.87$ cm s^{-1}. Therefore, the flow rate q per unit width and the mean velocity of flow are: $q = 53/[(60)(18.5)] = (4.77)(10^{-2})cm^3 s^{-1}$cm^{-1} and $w_{av} = (2/3)(1.87) = 1.24$ cms^{-1}. Depth of liquid hence becomes: $h = q/w_{av} = (4.77)(10^{-2})/1.24 = (3.83)(10^{-2})$ cm. For thin biofilms, biological efficiencies do

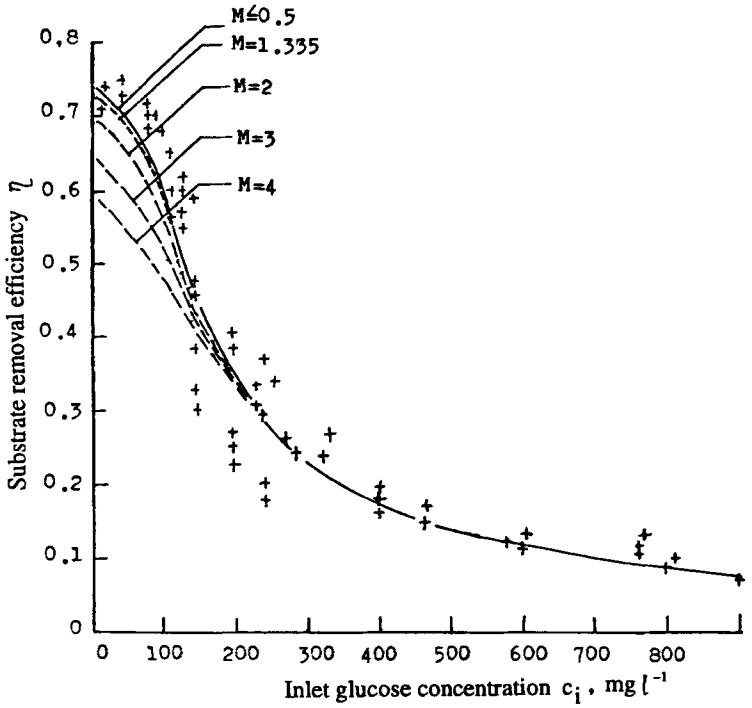

Fig. 6. Variation of substrate removal efficiency η with dimensionless biofilm thickness M and inlet glucose concentration c_i. Data of Atkinson and How, 1974 (5).

not depend on the dimensionless biofilm thickness M, when the chosen value of M is sufficiently small (The effect of M on η will be studied later). Therefore, selecting an arbitrary biofilm thickness M and using an estimated k_3 value, biological efficiency η is calculated from the computer program developed as a function of c_i and compared with the measured values. If an agreement exists between the theoretical and experimental results, the estimated value of k_3 is correct. Otherwise the above-mentioned procedure should be repeated. The result of the final trial will be given below for the sake of illustration. In the final trial, a best fit value of $k_3 = 1.18 \times 10^5$ cm^3 g^{-1} was obtained and a dimensionless biofilm thickness of $M = k_2 L = 0.1$ was used. Computer input data were first determined from the known asymptotic conditions. For large concentrations, the relationship of η vs c_i is reduced to Eq. (38) as mentined before. The value of $k_1 L$ was then obtained from this asymptotic condition. For this purpose, a graph of η vs $1/c_i$ was plotted from the experimental results. The first portion of this graph is a straight line with a slope of

$$\text{Slope} = (k_1 L / k_3)(\ell / q) = (7.5)(10^{-5})\, g\ \text{cm}^{-3} \tag{40}$$

Inserting the given data into Eq. (40) yields

$$k_1 L = (7.5)(10^{-5})(1.18)(10^5)(4.77)(10^{-2}) / (223.5) \tag{41}$$
$$= (1.892)(10^{-3})\ \text{cm}^3 s^{-1} \text{cm}^{-2}$$

Dimensionless filter length α was calculated using Eq. (33) as

$$\alpha = (k_1L / k_2L)\,(\ell / q) = [(1.892)(10^{-3}) / (0.1)]\,[223.5 / (4.77)(10^{-2})] = 88.65 \quad (42)$$

Mass transfer coefficient E can now be obtained from Fig. 3 using a molecular diffusion coefficient of $D_w = (6.9)(10^{-6})$ $cm^2 s^{-1}$ for glucose solution as follows:

$$Z_D = D_w \ell / h^2 w_{max} = (6.9)(10^{-6})(223.5) / [(3.83)(10^{-2})]^2\,(1.87) = 0.562 \quad (43)$$

$$\eta_D = (k_1L / D_w)\,h = [(1.892)(10^{-3}) / (6.9)(10^{-6})]\,(3.83)\,(10^{-2}) = 10.5 \quad (44)$$

$$e / h = 0.517\,; e = (0.517)(3.83)(10^{-2}) = (1.98)(10^{-2})\ cm \quad (45)$$

$$E = D_w / e = (6.9)(10^{-6}) / (1.98)(10^{-2}) = (3.485)(10^{-4}) \quad (46)$$

$$K = (k_2L / k_1L)\,(D_w / e) = [0.1 / (1.892)(10^{-3})].\ [(6.9)(10^{-6}) / (1.98)\,(10^{-2})] = 0.0185 \quad (47)$$

The other values necessary for performing the computer program are:

$$A_1 = (10^{-6})\,k_3 = (10^{-6})(1.18)(10^5) = 0.118\ cm^3 g^{-1} \quad (48)$$

$$A_o = (k_2 / k_1)\,q = (k_2L / k_1L)\,q = [0.1 / (1.892)(10^{-3})].\ (4.77)(10^{-2}) = 2.521\ cm \quad (49)$$

The computer program was performed using these input data. Values of η obtained as computer output were also plotted in Fig. 6 against c_i. The solid line in Fig. 6 was obtained. The predicted concentrations are in good agreement with the measured values. The solid line corresponding to the computer results fits the experimental points best. Therefore, the value of k_3 used in the calculation is correct.

In order to determine the effect of M on substrate removal efficiency η, the procedure explained above were repeated for $M = 0.3$, $M = 0.5$, $M = 1.25$, $M = 1.335$, $M = 2.0$, $M = 3.0$, and $M = 4.0$. The computer output were also plotted in Fig. 6 against c_i. A study of the computer results indicates that η values for the same inlet concentrations c_i are different from each other not more than 1% when $M < 1.25$. Deviations are even smaller than 0.5% for $M < 0.5$ (*see* Fig. 6). Therefore computer outputs obtained for $M = 0.1$ give the substrate removal efficiencies η for a thin biofilm and assumptions made are correct.

SUMMARY AND CONCLUSIONS

Mass transfer within microbial films is described using Monod-type biological kinetics in terms of the properties of packing material and feed solutions (*6*). For this purpose, computer techniques were first developed for the numerical evaluation of the normalized biofilm mathematical model. A second-order partial differential equation describing the mechanism of axial dispersion inside the liquid layer was then solved using method of finite differences to determine the mass transfer coefficient.

The results were plotted in terms of dimensionless filter length and dimensionless liquid depth incorporating with diffusion coefficient and kinetic parameters. The vaidity of the model and the derived equations were demonstrated by experimental results from the literature.

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APPENDIX A

Determination of the Biological System Parameters After Atkinson and Davies, 1974 (*4*)

$$\lambda = 1 - (\tanh k_2L / k_2L)\,[(\phi / \tanh \phi) - 1] \text{ for } \phi \leq 1 \quad \text{(A1)}$$

$$\lambda = (1 / \phi) - (\tanh k_2L / k_2L)\,[(1 / \tanh \phi) - 1] \text{ for } \phi \geq 1 \quad \text{(A2)}$$

in which

$$\phi = k_2L / (1 + 2k_3c_s)^{1/2} \quad \text{(A3)}$$

APPENDIX B

Derivation of Eq. (31)

Inserting Eq. (5) into Eq. (29) and using the dimensionless variables $M=k_2L$ and $B=k_3c$, it results that

$$dB / dZ = - K(B - B_s) = - g \tag{B1}$$

or

$$B = B_s + g / K \tag{B2}$$

in which

$$K = Ek_2 / k_1 \tag{B3}$$

$$g = \lambda M B_s / (1 + B_s) \tag{B4}$$

$$Z = (k_1 / k_2)(z / q) = z / A_o \tag{B5}$$

$$A_o = (k_2 / k_1) q \tag{B6}$$

The dimensionless filter length $\overline{Z}$ in which dimensionless substrate concentration is reduced from any inlet concentration of B_{si} (or B_i) to a given outlet concentration $\overline{B}_{so}$ (or $\overline{B}_o$) is obtained from

$$\overline{Z} = \int_{B_{so}}^{B_{si}} F \, dB_s \tag{31}$$

in which

$$F = (1 / g)[1 + (1 / K)(dg / dB_s)] \tag{B8}$$

For large values of c_s, as an asymptotic condition, $\lambda \rightarrow 1$ and $g \rightarrow M$ are obtained from Eqs. (A1) and (A2). Integration of Eq. (B1) then leads to

$$B_i - B_o = M \alpha \tag{B9}$$

which gives Eq. (38), if dimensional quantities are substituted.

APPENDIX C

Let us calculate η for an influent substrate concentration $B_i = 0.2009$ for the data given in the heading of Table 1. The values of B_{si} and $\overline{Z}_i$ in Table 1 corresponding to a given inlet concentration $B_i = 0.2009$ are $B_{si} = 0.0450$ in column 1 and $\overline{Z}_i = 15.3290$ in column 7. Since the dimensionless filter depth is given as $\alpha = 6.6374$ in the heading of Table 1, the value of $\overline{Z}$ corresponding to the outlet of filter becomes $\overline{Z}_o = \overline{Z}_i - \alpha = 15.3290 - 6.6374 = 8.6916$.

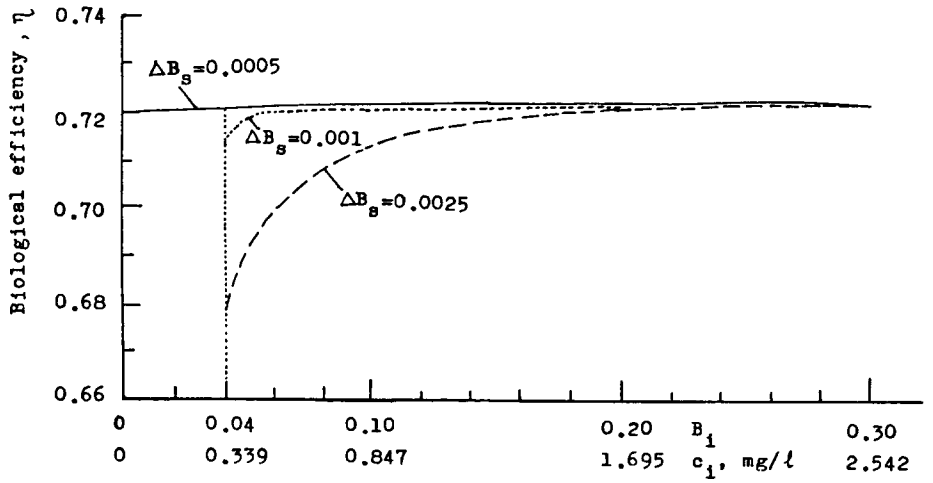

Fig. 7. The effect of increment $\triangle B_s$ on biological efficiency η ($M=1.3350$; $K=0.2480$; $A_1=0.1180$ cm^{3}g^{-1}; $A_o=33.673$ cm; $\alpha=6.6374$).

The dimensionless outlet concentration B_o corresponding to the value of $\overline{Z}_o=8.6916$ is obtained through linear interpolation as $B_o=0.0560$ from the values written in columns 4 and 7 in Table 1. The biological efficiency hence becomes $\eta=1-(B_o/B_i)=1-(0.0560/0.2009)=0.721$ for the inlet concentration of $B_i=0.2009$ (or $c_i=B_i/A_1=0.2009/0.118=1.702$ mg ℓ^{-1}). The calculated values of c_i and η are written in columns 9 and 10 of Table 1 in the same line as $B_{si}=0.0450$. The above mentioned calculations are included in the computer program developed.

Only the first portion of the computer output is shown in Table 1 that includes the results for $c_i<1.702$ mg^{L-1}. η values obtained from the computer program that are not included in Table 1 are plotted in Fig. 6 against c_i. A study of Fig. 6 indicates that substrate removal efficiency η decreases with the increasing value of inlet concentration c_i. For $c_i\rightarrow 0$, η is practically constant, (e.g., 0.721 in Fig. 6) although there is a slight change in η with small fluctuations owing to the step by step performance of the numerical integration (*see* Fig. 7).

In order to determine the effect of $\triangle B_s$ on biological efficiencies, the computer program has been modified to obtain the results for the selected values of B. For purpose of comparison, η values have been obtained for three different increments of $\triangle B_s=0.0025$, $\triangle B_s=0.0010$, and $\triangle B_s=0.0005$ as an example in Fig. 7. A study of Fig. 7 indicates that η values change not more than 0.1% for $\triangle B_s\leq 0.001$. It means that concentration increments smaller than $\triangle B_s=0.001$ do not practically effect η. Therefore computer programs were performed using a concentration increment of $\triangle B_s=0.001$ for all calculations in this study.