J. Indian Chem. Soc.,
Vol. 96, December 2019, pp. 1529-1538

A simplified approach for modelling of an aerobic fixed bed hybrid bioreactor

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Manuscript received online 21 August 2019, revised 01 December 2019, accepted 02 December 2019

A simplified model pertaining to the process design of an aerobic fixed bed hybrid bioreactor has been developed in a user-friendly manner. It is based on mass balance of both carbonaceous substrate and biomass under suspended and attached growth simultaneously along with substrate mass transport into the biofilm. Monod kinetics is followed for the utilization of carbonaceous substrate assuming no inhibition. The novelty in this analytical solution lies in determination of the average substrate flux considering varying substrate concentration profile inside the biofilm.The determination of effective biofilm thickness (L_e) has also been possible in this simplified model, which otherwise was not found in earlier existing ones. FORTRAN computer program is developed for obtaining the necessary outputs and the model has been validated with both the existing methods of standard literatures as well as with the experimental results. It is found a quick, easy and simpler than the existing methods.

Keywords: Hybrid bioreactor, activated sludge-biofilm modeling, Monod kinetics, FORTRAN program, model performance.

Introduction

Hybrid bioreactor carrying both suspended-growth and attached-growth microorganisms has been found a novel and excellent bioreactor system for treating the wastewater containing easily biodegradable substrates. In order to design a hybrid biological process, a rational and simplified model is very much useful. Hybrid bioreactor model is essentially based on integration of both the suspended and attached growth kinetics, where two types of microorganism act simultaneously. There is a limited number of method available for solving problems on hybrid bioreactor system. Solution of biofilm models is much tedious and cumbersome compared to the suspended growth. The reliable analysis for predictions pertinent to the performance of the said reactor is still unavailable. Most kinetic models assumed single growth i.e. either suspended or attached in sequential fashion. Even where the competition for rate limiting substrates between two growths (both suspended and attached) were simultaneously considered, no unique accurate and simplified solution was derived from the steady state substrate mass balance and biomass balance equations.

Various researchers have developed their model on hybrid bioreactor, which have certain limitations. In the earlier research, one steady state substrate balance for both suspended and attached growth and the biomass balance for the suspended growth were used to develop a model for the hybrid bioreactor considering both attached and suspended growth simultaneously[1]. The drawback of this model was that the Regular-Falsi method was applied for the numerical solution of the said model and was found inconvenient and approximate too. One computer program was developed for integrated fixed film activated sludge system for removing soluble COD and nutrients[2]. However, the model was found very complicated without considering the simultaneous growth of both suspended and attached biomass. Later hybrid bioreactor model was applied in a typical activated sludge process, where, biofilm was provided with plastic nets vertically inside the tank[3,4]. The combination of suspended and attached biomass enhanced effluent concentration, solids settling and improved nitrification efficiency. The drawback of the model was that suspended and attached growth were not considered simultaneously instead initially attached

growth and subsequently suspended growth was simulated.

In order to analyze an aerobic fixed bed hybrid process, a simplified mathematical model was developed for a steady state biofilm activated sludge reactor to calculate the substrate flux in the biofilm under substrate limiting condition (Bhargava *et al.*, 2004). However, the solution of the mathematical model can be done only if the effluent substrate concentrationis already assigned a value, i.e. for a desired effluent substrate concentration the model determines the substrate flux. One activated sludge model (ASM2d) was developed for biological phosphorus removal with simultaneous nitrification-denitrification in ASP[5]. The said model was further extended to a steady state Integrated Fixed Film Activated Sludge (IFAS) model[6] with the input taken from biofilm modelling techniques[7]. The said IFAS model considered competition between the biofilm and suspended biomass for macronutrients, electron donor and electron acceptor substrates. The theoretical considerations in the said model include simultaneous diffusion and Monod type reaction kinetics inside the biofilm. The drawback of this IFAS model is that the biofilm thickness L_f is to be known as a priori to run the analysis and the fate of soluble COD is poorly understood.

In view of all such constraints and limitations, a simplified model for aerobic fixed bed hybrid bioreactor is thus developed to easily calculate the output parameters like exiting substrate concentration in bulk liquid, average substrate flux in the biofilm, effective and total biofilm thickness.

Model description

The concept diagram of a typical fixed bed hybrid bioreactor comprising of activated sludge-biofilm is shown in Fig. 1.

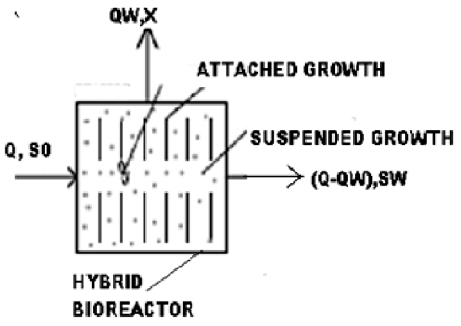

Fig. 1. Schematic diagram of a hybrid bioreactor.

In the above system a portion of substrate is uniformly exposed to the suspended biomass. The remaining fraction of substrate flows through the biofilm-liquid interface and then through the biofilm as shown in Fig. 2.

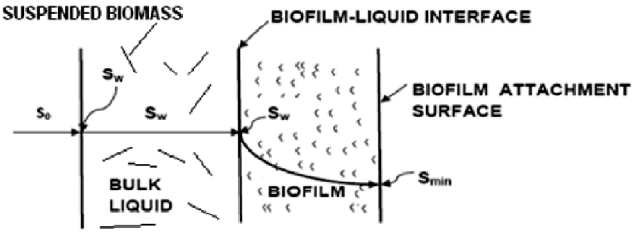

Fig. 2. Profile of substrate concentration in a hybrid bioreactor.

From the steady state substrate balance for both the suspended growth and attached growth the following equation can be obtained.

$$S_0 - S_w - \frac{pkXS_w\theta}{K + S_w} - aJ_{avg}\theta = 0 \qquad (1)$$

where, S_0 = entering substrate concentration (mg/cm^3), S_w = exiting substrate concentration (mg/cm^3) in the bulk liquid, p = porosity of hybrid reactor, k = maximum specific rate of substrate utilization (per day), X = concentration of suspended biomass in hybrid reactor (mg/cm^3), θ = empty bed hydraulic detention time (h), K = half velocity coefficient (mg/cm^3), a = specific surface area of supporting media (cm^{-1}) and J_{avg} = average substrate flux into the biofilm (mg/cm^2/day).

To calculate the average value of "substrate flux" (J_{avg}) into the biofilm, 5 (five) divisions (based on equal interval of substrate concentration) inside the biofilm have been considered as shown in Fig. 3. Such an arrangement of divisions is conceptualized within the biofilm for determining the accurate value of individual substrate flux at respective division. It has also been observed that there is hardly any deviation of results in case number of divisions is more than five (5).

$J_{avg} = (J_0 + J_1 + J_2 + J_3 + J_4 + J_5)/6$, (Sarkar and Mazumder[8]), where, J_1, J_2, J_3 , J_4 and J_5 are substrate flux corresponding to substrate concentration S_1, S_2, S_3, S_4 and S_w respectively. J_0, the substrate flux corresponding to S_{min} is zero. Now, J, the substrate flux can be determined from the solution of mass balance equation of substrate in biofilm,

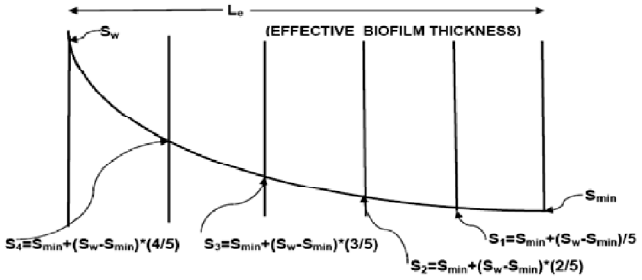

Fig. 3. Divisions in substrate concentration profile within the biofilm.

i.e. $\frac{d^2S_f}{dz^2} = \frac{kX_fS_f}{D_f(K + S_f)}$ as follows:

$$J = \sqrt{2kX_fD_f[(S_{entry} - S_{exit}) + K\ln[(K+S_{exit})/(K+S_{entry})]}} \quad (2)$$

where, S_f = substrate concentration at any point in the biofilm (mg/cm^3), X_f = active biomass density within the biofilm (mg/cm^3), D_f = molecular diffusion coefficient of the substrate in the biofilm (cm^2/day), S_{entry} = entering substrate concentration in a small segment in the biofilm and S_{exit} = exiting substrate concentration in a small segment in the biofilm.

$$S_{min} = K \times \frac{b_t}{Y \times k - b_t}$$

where, S_{min} = minimum concentration of rate-limiting substrate at biofilm-attachment surface (mg/cm^3).

Now, from the steady state mass balance of active micro organisms in a biofilm, as well as under suspended growth state.

$$\frac{YaJ_{avg}}{pX}\frac{b_s}{b_t}\frac{1}{\theta_c} + \frac{YkS_w}{K + S_w} - b_d = 0$$

$$\text{i.e. } X = \frac{YaJ_{avg}\frac{bs}{pbt}}{\frac{1}{\theta_c} + b_d - \frac{YkS_w}{K+S_w}} \quad (3)$$

where, Y = bacteria yield coefficient, b_s = biomass loss rate due to shearing from biofilm, day^{-1}, b_t = total biomass loss rate from biofilm, day^{-1}, b_d = biomass decay coefficient, day^{-1} and θ_c = mean cell residence time or solid retention time.

Putting the value of X in eq. (1), we get,

$$S_0 - S_w - \frac{kS_w\theta YaJ_{avg}\frac{b_s}{b_t}}{(K+S_w)\left(\frac{1}{\theta_c} + b_d - \frac{YkS_w}{K+S_w}\right)} - aJ_{avg}\theta = 0 \quad (4)$$

The eq. (4) can be reformed as,

$$S_0 - S_w - A1J_{avg} - aJ_{avg}\theta$$

$$\left[\text{considering } A1 = \frac{kS_w\theta Ya\frac{b_s}{b_t}}{(K+S_w)\left(\frac{1}{\theta_c} + b_d - \frac{YkS_w}{K+S_w}\right)}\right]$$

$$\text{i.e., } S_0 - S_w = J_{avg}(A1 + a\theta) \quad (5)$$

Now, from eqs. (1) and (5), by process of iteration in a computer program (FORTRAN), S_w, the exiting substrate concentration in the bulk liquid can be determined (For the detail programthe authors may kindly be referred).

Now, for calculating the effective biofilm thickness L_e, applying Runge-Kutta method, solution of equation

$\frac{d^2S_f}{dz^2} = \frac{kX_fS_f}{D_f(K + S_f)}$ can be used as follows:

$$\frac{d^2S_f}{dz^2} = f\left(Z, \frac{dS_f}{dz}\right), \frac{dS_f}{dz}(Z_0) = \frac{dS_{f0}}{dz} = K1 = 0$$

$$[S_{f0} = S_{min} \text{ at } z = 0]$$

$$L1 = f\left(Z_0, \frac{dS_{f0}}{dz}\right) = \frac{d^2S_{f0}}{dz^2} = \frac{kX_fS_{f0}}{D_f(K + S_{f0})}$$

$$\frac{dS_{f1}}{dz} = \frac{dS_{f0}}{dz} + 0.5 \times L1 \times h = K2,$$

where h = step = effective biofilm thickness (cm), h is the distance between z = 0 (at the attachment surface) and z = L_e (at the biofilm/water interface)

$$L2 = h \times f\left(Z_0 + \frac{h}{2}, \frac{dS_{f1}}{dz}\right) = h \times \frac{d^2S_{f1}}{dz^2}$$

$$= \frac{kX_f(S_{f0} + 0.5K1 \times h}{D_f(K + S_{f0} + 0.5K1 \times h}$$

$$\frac{dS_{f2}}{dz} = \frac{dS_{f0}}{dz} + 0.5\times L2\times h = K3,$$

$$L3 = h\times f\left(Z_0 + \frac{h}{2}, \frac{dS_{f2}}{dz}\right) = h\times\frac{d^2S_{f2}}{dz^2}$$

$$= \frac{kX_f(S_{f0} + 0.5K2\times h}{D_f(K + S_{f0} + 0.5K2\times h}$$

$$\frac{dS_{f3}}{dz} = \frac{dS_{f0}}{dz} + L3\times h = K4,$$

$$L4 = h\times f\left(Z_0 + h, \frac{dS_{f3}}{dz}\right) = h\times\frac{d^2S_{f3}}{dz^2}$$

$$= \frac{kX_f(S_{f0} + K3\times h}{D_f(K + S_{f0} + K3\times h}$$

$$\Delta Y(1) = \frac{h}{6}\times(K1 + 2\times K2 + 2\times K3 + K4) \quad (6)$$

$$\Delta Y(2) = \frac{h}{6}\times(L1 + 2\times L2 + 2\times L3 + L4) \quad (7)$$

Here, $\Delta Y(1)$ stands for increment of substrate concentration, $\Delta Y(2)$ stands for $\frac{dS_f}{dz}$

Therefore,

$$S_w = S_{min} + \Delta Y(1) \quad (8)$$

$$J5 = D_f\times\Delta Y(2) \quad (9)$$

Again,

$$L_f = \frac{J\times Y}{X_f\times b_t}, \text{ where } L_f = \text{total biofilm thickness (cm)} \quad (10)$$

In order to calculate S_w, J and L_e using eqs. (1), (2), (3), (4), (5), (6) and (7), i.e. to solve the hybrid bioreactor model, two flowcharts were constructed as shown in Fig. 4 and Fig. 5. Consequently, two detailed FORTRAN programs have been developed on the basis of those flowcharts (for detailed program corresponding author may kindly be referred.

Essence of flowcharts constructed

Two flowcharts for computer programming in FORTRAN have been prepared approaching the iteration processes, with a view to calculate unknown exiting substrate concentration S_w, average substrate flux J_{avg} (Fig. 4) and effective biofilm thickness L_e (Fig. 5). In the first flowchart, eqs. (1), (2), (3), (4) and (5) as stated earlier are simultaneously iterated to calculate the unknown exiting i.e. bulk liquid substrate concentration S_w and unknown flux J. The initial iteration value S_w was assumed in this flowchart as any value higher than S_{min} (which is required to sustain a steady biofilm growth). The second flowchart utilized the value of S_w as obtained from the flowchart 1 to calculate L_e following the concept of Runge-Kutta method of analysis. The convergence of iteration was attributed at the liquid/biofilm interface when computed substrate concentration (S_w) becomes equal to the assumed one.

Modality of application of the developed model

The solution method derived from the proposed model can be applied to determine the exiting substrate concentration i.e. bulk liquid substrate concentration (S_w) and the average substrate flux (J_{avg}) by running the FORTRAN program based on the flowchart as shown in Fig. 4. After determination of the values of S_w and J_{avg}, the FORTRAN program based on the flowchart as shown in Fig. 5 can be run for evaluating both the total and effective biofilm thickness L_f and L_e.

Experimental validation of the developed model

In order to find out the accuracy of the developed model, one laboratory scale hybrid bioreactor set-up was run under continuous mode using synthetic carbonaceous wastewater. The said reactor comprised of both the suspended growth biomass as well as attached microorganism in the biofilm media. The reactor was run under continuous mode to validate the proposed model.

Description of an aerobic hybrid bioreactor setup

A 12 litre capacity PVC jar has been used to fabricate the laboratory-scale hybrid bioreactor set-up. Perspex sheet (3 mm thickness) was taken as attachment surface for the growth of biomass. Nine equal slots each of 40 degree and height of 275 mm perspex sheets are combined together as shown in the Fig. 1 and inserted in the jar with a gap of 1 inch from bottom surface of the jar for maintaining the sludge growth at bottom. Total fixed surface area for attachment of biomass is 0.27 sqm, where as thetotal varying surface area for attachment was 0.132 sqm. A mild steel box was in-

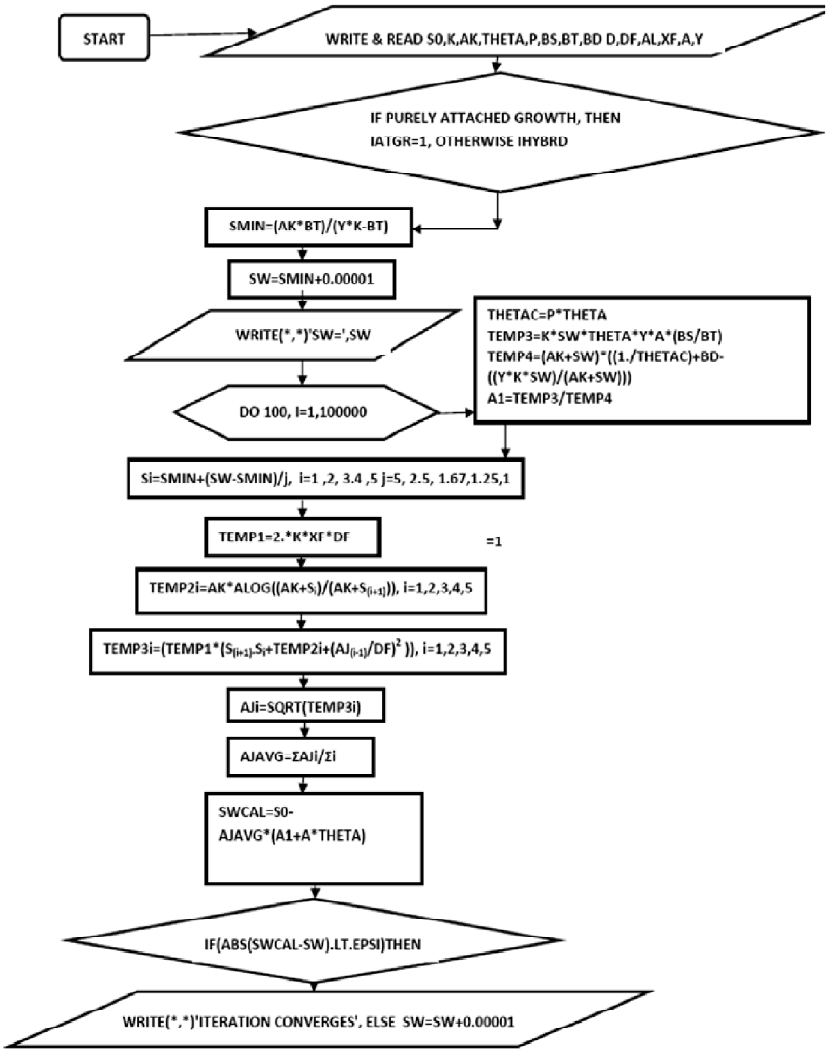

Fig. 4. Flowchart for programming in FORTRAN to calculate unknown exiting substrate concentration S_w and average substrate flux J_{avg}.

stalled on the top of the jar through which eight (8) nos. 10 mm dia. CPVC pipes were vertically placed for the sake of operation. One sludge outlet perpendicular to the direction of inlet-outlet line was fitted at bottom of the reactor. Outlet pipe emerging from the reactor was extended to the secondary clarifier which was placed in a PVC vessel for collecting the overflow from the secondary clarifier.

Composition of synthetic wastewater

Experimental procedure

A synthetic carbonaceous wastewater was used as a stock solution, where, COD concentration was set to about 1000 mg/L. Adequate nitrogen and phosphorus were also added to this stock solution in accordance with carbon. Variable initial COD concentrations were set by diluting the stock solution with distilled water. The composition of stock synthetic solution is shown in Table 1.

The hybrid bioreactor set-up was run under continuous mode with initial COD concentrations viz. 150, 200 and 250 mg/L and maintaining a HRT of 4, 6 and 8 h. The initial biomass concentration (both suspended and attached) was also varied as perinitial COD concentration. The reactor was allowed to run by means of peristaltic pump until quasi-steady state condition reached. The effluent sample was taken for

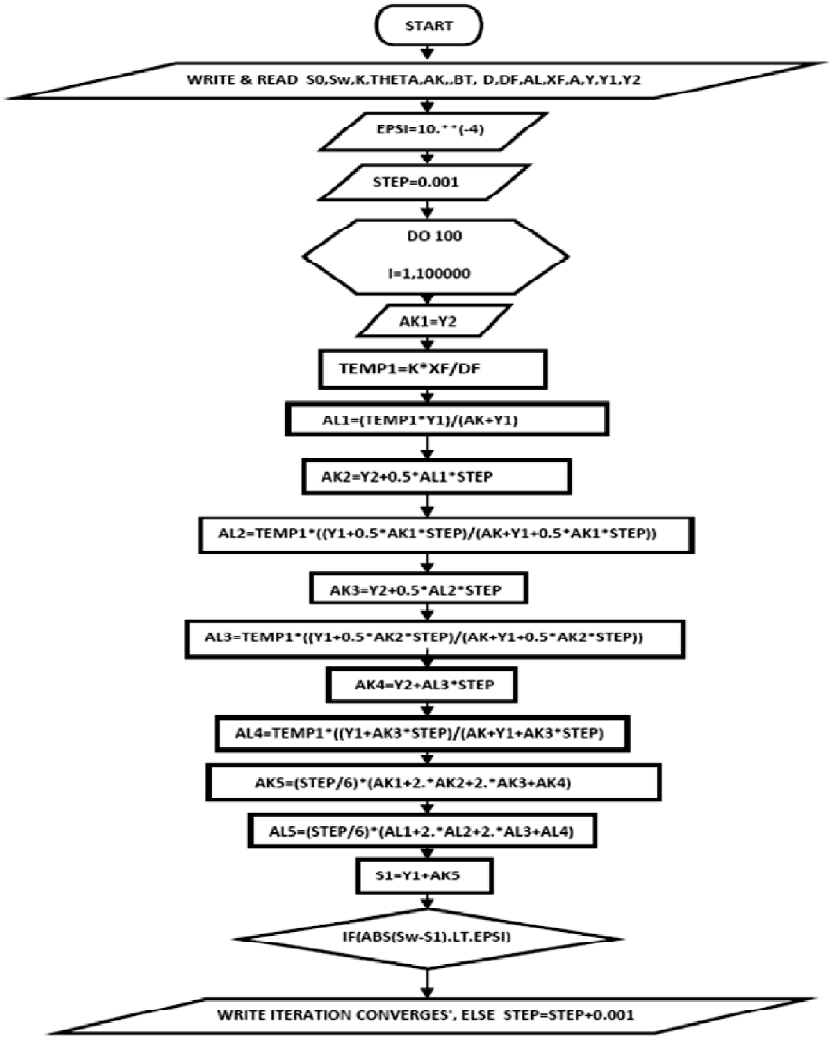

Fig. 5. Flowchart for programming in FORTRAN to calculate effective biofilm thickness (L_e) under a known exiting substrate concentration (S_w).

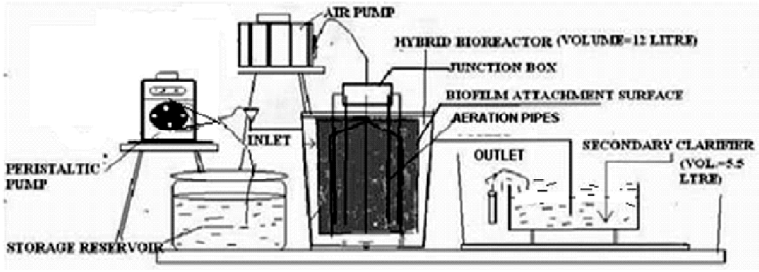

Fig. 6. Schematic diagram of a fixed film aerobic ybrid bioreactor under continuous mode of operation.

Table 1. Composition of synthetic wastewater with COD concentration 1000 mg/L (appx.)

Compound	Concentration (mg/L)
Dextrose ($C_6H_{12}O_6$)	940
NH_4NO_3	260
KH_2PO_4	82.67
$CaCl_2$	27.5
$MgSO_4.7H_2O$	22.5
$FeCl_3$	0.25

measuring final COD concentration, where as the reactor content was taken for determining steady state suspended biomass concentration. A portion of attached media (perspex sheet) was washed out with 1 *N* NaOH solution to measure the attached biomass.

Method of analysis

All the parameters except the attached biomass were measured as per Standard methods (1995). The attached biomass was determined from the protein measurement following Lowry's method (1950) modified by Herbert *et al.* (1972).

Results of analysis

The proposed model for the hybrid bioreactor was used to determine the relevant output parameters analytically under the different sets of input parameters. The effluent substrate concentration (S_w), the substrate flux (J), the effective biofilm thickness (L_e) and the total biofilm thickness (L_f) were considered as the output parameters. The analytical solution by the proposed model is designated as Case 1. The same analytical solution has been compared with the solution using different existing methods as demonstrated in available literatures to judge the efficacy of the proposed model. The model analysis by Lee[1], Fouad and Bhargava[9] and Gebara[3], are denoted as Case 2, Case 3 and Case 4 respectively. Table 2 illustrates the comparison of output parameters between Case 1 and Case 2, 3 and 4 separately. In the comparison analysis, all necessary kinetic coefficients and input parameters like initial substrate concentration (S_0), hydraulic retention time (θ), sludge retention time (θ_c), specific surface area (a) and attached biomass density (X_f) are chosen as per the standard literatures of the respective cases.

The results of analysis as shown in Table 2 depicted the outcomes from computer programming of the proposed

Table 2. Comparison of output parameters (S_s, J and L_e) using various hybrid bioreactor models

Data set No.	S_0 (mg/cc)	θ (h)	θ_c (h)	a (cm^{-1})	X_f (mg/cc)	S_w (mg/cc)		J (mg/cm^2/day)		L_e (cm)		L_f (cm)	
						Case 1	Case 2	Case 1	Case 2	Case 1	Case 2	Case 1	Case 3
1.	0.43	24	12	0.9	25	0.004	0.0039	0.271	0.2785	0.0104	***	0.012	0.0122
2.	0.43	12	12	1.8	25	0.004	0.004	0.27	0.28	0.0104	***	0.012	0.0123
3.	0.16	12	12	0.154	54.63	0.08	0.07	0.79	***	0.07	***	0.13	***

Note: Three star marks indicate that the values could not be obtained using the respective models.

Case 1: By proposed hybrid model.

Case 2: Proposed by Lee, 1992 using Ragular-Falsi method.

Case 3: Proposed by Fouad and Bhargava, (2004) using algebraic expression with dimensionless parameters.

Case 4: Proposed by Gebara, 1999 using the reactor as composed of two reactors (biofilm and suspended) in series.

The kinetic co-efficients and physical data for comparison between Case 1 and Case 2, Case 1 and Case 3 are considered as follows: $k = 10\ day^{-1}$, $Y = 0.45$, $K = 0.01\ mg/cm^3$, $b_t = 0.41\ day^{-1}$, $b_s = 0.21\ day^{-1}$ $b_d = 0.2\ day^{-1}$ $D = 1.25\ cm^2/day$, $D_f = 0.75\ cm^2/day$, $L = 0.0078$ cm. The kinetic co-efficients and physical data for comparison between Case 1 and Case 4 is considered as: $k = 2.08\ day^{-1}$, $Y = 0.72$, $K = 0.087\ mg/cm^3$, $b_t = 0.08\ day^{-1}$, $b_s = 0.04\ day^{-1}$, $b_d = 0.04\ day^{-1}$, $D = 1.25\ cm^2/day$, $D_f = 0.393\ cm^2/day$, $L = 0.0078$ cm.

model which were compared with the existing models. The results of the continuous study on hybrid bioreactor are presented in Table 3.

In order to check the accuracy of the proposed model, experimental COD values were plotted with respect to the COD values predicted from the present model as shown in Fig. 7. It has been observed that all the experimental results are approximately within (±) 10% deviation from the model outputs.

Table 3. Comparison of effluent substrate concentration (S_w) with the experimental data (obtained from continuous studies)

Influent COD, S_0 (mg/L)	Effluent COD, S_w (mg/L) from experiment	HRT, θ (h)	Predicted COD, S_w (mg/L) from the proposed model	% Deviation
150	20	8	21	5
150	43	6	45	4.45
150	75	4	74.8	0.26
200	21	8	21	0
200	45	6	47.00	4.44
200	87	4	80	8.75
250	24	8	22	9
250	49	6	48	2.04
250	88	4	83	5.68

The kinetic co-efficients and physical data used for prediction of the effluent substrate concentration are as follows: k = 1.24 day^{-1}, Y = 0.5, K = 0.04 mg/cm^3, b_t = 0.08 day^{-1}, b_s = 0.04 day^{-1}, b_d = 0.04 day^{-1}, D = 0.8 cm^2/day, D_f = 0.64 cm^2/day, L = 0.01 cm.

Results and discussion

Three input data sets were used to determine the effluent substrate concentration (S_w), the substrate flux (J), the effective biofilm thickness (L_e) and the total biofilm thickness (L_f) in Case 1, Case 2, Case 3 and Case 4. The effluent substrate concentration as determined by the proposed model (Case 1) satisfactorily tallied with that from Case 2 (Lee[1]) and Case 4 (Gebara[3]). It is to observe that, it exactly equals to S_w obtained from Case 3 (Fouad and Bhargava[9]), when data set 2 was used. As a whole, there is hardly any discrepancy between the proposed model and the other existing models in respect of effluent substrate concentration. In addition, the proposed model solution is much simpler than the existing ones and needs a short time.

The substrate flux (J), obtained by the proposed model is also in a very good agreement with that obtained from Case 2 and Case 3 for two input data sets. Since the substrate flux was not determined by Gebara[3] in Case 4, it could not be compared with Case 1. Out of Case 2 (Lee[1]) and Case 3 (Fouad and Bhargava[9]), the value of J from the proposed model is more converging in Case 2. Indeed the methods of determination J in Case 2 and Case 3 are complicated and also approximate. It has also been explored that the sub-

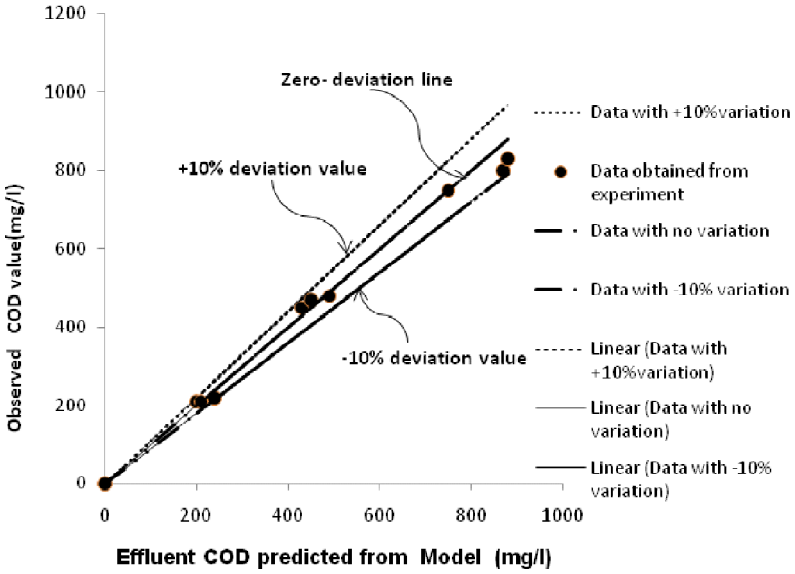

Fig. 7. Plotting of predicted and observed COD concentrations.

strate flux (J) could be determined in a limited cases. In view of that the proposed model established a simple mechanism for determining the substrate flux into the biofilm in a hybrid bioreactor.

The effective biofilm thickness (L_e) was not measured previously by Lee[1] (Case 2), Fouad and Bhargava[9] (Case 3) and Gebara[3] (Case 4). The proposed model (Case 1) only could determine the effective biofilm thickness and their values appeared to be reliable. Although, the effective biofilm thickness was found to be same for data set 1 and 2, it is only due to simultaneous variation of two input data. The effective biofilm thickness was always observed to be less than the total biofilm thickness.

The total biofilm thickness (L_f) as obtained by the proposed model almost equals to that determined from Case 2 and Case 3. It clearly demonstrates the accuracy of the proposed model in respect of total biofilm thickness. However, L_f, calculated from the proposed model could not be compared with Case 4, because no such information is available.

The results of continuous study in terms of soluble COD concentration are within ±10% variation with respect to the model output. It is also to note that more than 50% observed COD data remain within ±5% variation. Since continuous study on a reactor system represents a realistic situation, its' results can be used for validation of the proposed model. On the basis of data comparison it can reasonably be informed that the proposed model is good enough for prediction of effluent COD (substrate) concentration in a hybrid bioreactor. In this regard, all the kinetic co-efficients have been derived from kinetic study on the same hybrid bioreactor with the same synthetic wastewater.

Conclusions

So far, a very few mathematical models of the hybrid bioreactor are developed considering the simultaneous growth of suspended and attached biomass. Simultaneous utilization of the substrate by suspended and attached biomass in a competitive manner is very much essential for process design of such reactor.

Although there is a number of analytical techniques for solving the mathematical model of hybrid bioreactor, all those are substantially approximate, complicated and tedious in nature. Thus a simplified model (with computer programming) for hybrid bioreactor finds its relevance for predicting the reliable outputs for the sake of process design. There is a flexibility of the proposed model making it a versatile one to find out the exiting substrate concentration both in hybrid bioreactor as well as in a completely mixed biofilm reactor. No approximation was considered in this proposed model depicting its uniqueness compared with the existing methods of numerical analysis. Apart from that, the developed model determined the substrate flux at any layer of the biofilm matrix along with the effective and total biofilm thickness. Compared to the analysis of the model of hybrid bioreactor developed by the past researchers, the proposed model is found very simple, fast and accurate in determining the output parameter required for the process design of hybrid bioreactor.

The performance results from a laboratory-scale hybrid bioreactor corroborate with the effluent COD concentration, predicted from the present model. The continuous study performed on this reactor under varying influent COD concentrations, HRT etc. clearly exhibited that the present model is applicable for variation in process parameters also. Hence, it may be successfully used in the process design of the hybrid bioreactor for a given set of physical data and relevant kinetic coefficients. The steady state suspended biomass in the hybrid bioreactor can also be determined using the present mathematical model, which is essential for subsequent sludge management strategy.

Acknowledgements

The authors would like to acknowledge their sincere thanks to Mr. Supriyo Goswami for his dedicated assistance in carrying out the present research work.

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