Soil Biotechnology Process Simulation using Computational Fluid Dynamics

Umesh Yeole[1], Pattanaik B. R.[2] and Shankar H. S.[3*]
Department of Chemical Engineering, Indian Institute of Technology Bombay,
Powai, Mumbai-400076, India. Fax: 091-22-5723480 / 5726895
E-mail: 1. - yeoleup@iitb.ac.in 2. - biblab65@yahoo.com 3. - hss@che.iitb.ac.in

Abstract:

Soil biotechnology (SBT)is a system for water renovation which makes use of a formulated media with culture of soil micro and macro-organisms to process water and wastewater. The process gives advantage in terms of applicability for very small to large scale; natural aeration, no moving parts except pumps, no sludge, no odor and all green environment. Computational Fluid Dynamics (CFD) is used to study the hydrodynamics as well as rate limiting features of the system. Simulations are performed for different configurations of the bioreactor and the results are compared with laboratory and field experimental data. It is shown that this CFD model can be used to predict behaviour of the process.
Keywords: Soil-bioreactor, wastewater renovation, COD removal, soil-column, permeability, large scale bioreactor, CFD.

1 Introduction

Soil Biotechnology (SBT) is a process for processing of organic and oxidisable matter. In this system fundamental chemical reactions of nature viz. respiration, mineral weathering and photosynthesis are integrated and synergised to bring about the process.

As per carbon cycle, water supports four billion ton live carbon while soil and land support 800 billion ton live carbon. Life evolved in water two billion years ago but moved out on to land impelled by the thermodynamic logic - that life longs for itself and evolution is about minimizing energy needs - that it takes roughly 500 kJ/g live carbon per year to support life in water, 26 kJ/g live carbon per year in soil compared to 3 kJ/g live carbon per year on land. But conventional waste processing uses water as medium contrary to the design of carbon cycle. So in SBT, processing is carried out in soil.

In SBT, respiration serves to bring about oxidation of organics and inorganics and therby substantially reduce oxygen demand, mineral weathering serves to regulate the environment to enable these reactions to occur at the desired rates while photosynthesis serves as a bio-indicator of process performance. (Pattanaik et al., 2003). In warm climates the system is open to atmosphere while in very cold climes suitable closures may be needed. If space is a limitation then multi-staged bioreactor system (biotower) can be used.

SBT houses an engineered ecology of formulated media containing selected micro and macro-organisms such as geophagus earthworm *Pheretima elongata*, bioindicator plants. Bioconversion takes place by bacterial processing of organics and inorganics wherein geophagus worms regulate bacterial population. Patents of Pattanaik et al. (2002, 2004) contain details of media, culture and additives. COD, BOD, suspended solids, color, odor, bacteria, coliforms are removed all in a single all green facility open to atmosphere. It is unlike land treatment which is space intensive and unlike constructed wetlands which engages aquatic ecology.

Fig. 1a shows a schematic of the setup for a batch process and Fig 1b shows the schematic of the cross-section of the bioreactor. During passage of fluid over the media, removal of suspended

*Address all correspondence to this author

Table 1: Gross and simplified chemistry of engineered chemical reactions at work during bio-filtration. (Pattanaik et al., 2003b)

Respiration

$(CH_2ON_xP_yS_zK_y)_n + nO_2 + nH_2O$
$= nCO_2 + 2nH_2O$ + Minerals (N, P, S, K) + Energy (2.1)

Photosynthesis

nCO_2 + 2nH_2O + Minerals (N,P, S,K) + Sunlight
$= [CH_2ON_xP_yS_zK_y]_n + nO_2 + nH_2O$ (2.2)

where x = 0.16 - 0.016; y = 0.01 - 0.001; z = 0.02 - 0.002;
Lower values for terrestrial and Higher values for aquatic productions

Nitrogen Fixation

$N_2 + 2H_2O$ + Energy = $NH_3 + O_2$ (in soil) (2.3)

$N_2 + 2H_2O$ + Light = $NH_3 + O_2$ (in water) (2.4)

Acidogenesis

$4C_3H_7O_2NS + 8H_20 = 4CH_3COOH + 4CO_2 + 4NH_3 + 4H_2S + 8H^+ + 8e^-$ (2.5)

Methanogenesis

$8H^+ + 8e^- + 3CH_3COOH + CO_2 = 4CH_4 + 3CO_2 + 2H_2O$ (2.6)

Adding 5 and 6 give overall biomethanation chemistry

$4C_3H_7O_2NS + 6H_20 = CH_3COOH + 6CO_2 + 4CH_4 + 4NH_3 + 4H_2S$ (2.7)

Mineral weathering

$CO_2 + H_2O = HCO_3^- + H^+$ (2.8)

Primary mineral + $CO_2 + H_2O = M^{+n}$ + nHCO_3^- + soil/clay/sand (2.9)

Nitrification

$NH_3 + CO_2 + 1.5O_2$ = Nitrosomonas + $NO_2^- + H_2O + H^+$ (2.10)

$NO_2^- + CO_2 + 0.5O_2$ = Nitrobacter + NO_3^- (2.11)

De-nitrification

$4NO_3^- + 2H_2O$ + energy = $2N_2 + 5O_2 + 4OH^-$ (2.12)

solids takes place by filtration and biological oxidation, dissolved organics by adsorption and/or biological oxidation. Natural aeration serves as the oxygen source. So mass transfer from liquid to solid and biological reactions characterize the device.

Table 1 summarizes the gross and simplified chemistry of the fundamental natural processes engineered in SBT. The soil processes work at mesophilic temperatures (20 45 ^{0}C) wherein the energy of respiration (Eqn. 2.1) is used to derive nutrients such as nitrogen from the environment as per Eqn. 2.3. Bio indicator plants serve to remove excess metabolites via. photosynthesis given by Eqn. 2.2. The chemistry of acidogenesis determines generation of acidity due to decomposition as given by Eqn. 2.5. In addition there could be acidity generation due to nitrification given by Eqn. 2.7 and carbonic acid equilibria as given by Eqn. 2.8. In SBT, formulated mineral additives to regulate pH of the environment is engaged and Eqn. 2.9 gives the chemistry of this weathering reaction; M^{+n} represents the nutrients released from primary minerals and soil/sand/clay are the byproducts of this weathering reaction taking place. Assimilation of nitrogen (assimilatory nitrate removal) and plant uptake as given by Eqn. 2.10, and 2.11 and denitrification as given by Eqn. 2.12 are involved in nitrogen control. These chemical equations serve to quantitate the inputs-outputs from SBT conversion process. (Pattanaik et al., 2003).

Many such plants are operational now for treatment of water containing BOD, COD, ammoniacal nitrogen, coliforms and odor. Field experience suggests the scope to improve the efficiency and to reduce the cost of these plants. Performance enhancement of the bioreactor can be obtained by avoiding flow mal-distribution to improve the contact of fluid with media.

In this work, we present modeling of bioreactor using computational fluid dynamics (CFD) solver Fluent 6.1. Earlier Pattnaik et al. (2003) used a mixed cell model. But performance of large scale devices depend on spatial distribution of fluid. CFD model is advantageous as it solves the conservation equations for total mass, momentum, energy and species mass fraction over the system domain, with specified conditions for space and time.[Ranade, 2002] CFD model for the bioreactor involves only one parameter permeability (or hydraulic conductivity) which could be different in different directions. As shown in the paper permeability could be estimated from RTD data. Thus,

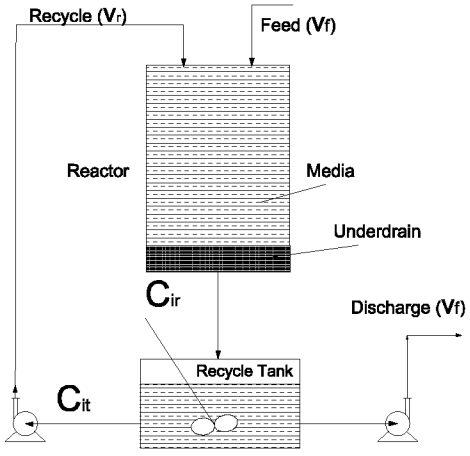
CFD provides a new tool to address large scale simulations. In this work we present CFD model and its validation.

The process uses one or more bioreactors and recycle tanks. CFD takes into account convective and diffusive supply of solute from liquid to solid phase. Darcy's law is used to represent sink term in the momentum balance wherein permeability (alpha) and its variation in the different directions are accounted. Species material balance with appropriate rate equations describe variation of concentrations of the species in the domain of interest. A Langmuir type isotherm is used to describe the equilibria between solid and liquid. The presence of recycle tank introduces a time lag which is accounted by suitable material balance.

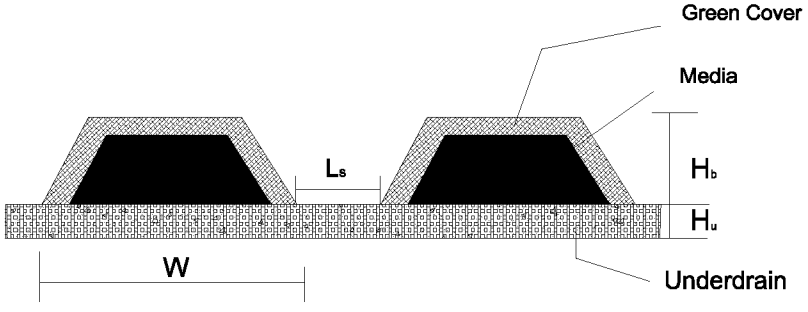
The model is simulated for laboratory and field scale devices. Important parameters controlling the process performance are rate constants, residence time of fluid in bioreactor, holding time in recycle tank and permeability of the media. Three cases are considered viz. 30 cm and 1.75 m deep cylindrical beds and commercial facilities.

Comparison of CFD simulations for batch experiments together with known kinetic parameters indicate that CFD model captures the features of the process very well. Comparison of CFD simulations with rates obtained in commercial facilities also show excellent agreement.

In conclusion we show that CFD is a powerful tool if parametrs of the fluid mechanics, biological reactions and transport processes kinetics are available and provides a focus on the parameter values needed for process performance.



(a) Schematic of experimental setup for biofiltration process. Here, C_{ir} is concentration of species at exit of reactor, C_{it} is concentraion of species in recycle tank



(b) Schematic of cross-section of field SBT bioreactor. Here, W is the width of media strench, H_b is the height of the media, H_u is height of underdrain.

Figure 1: Schematic of SBT Bioreactor

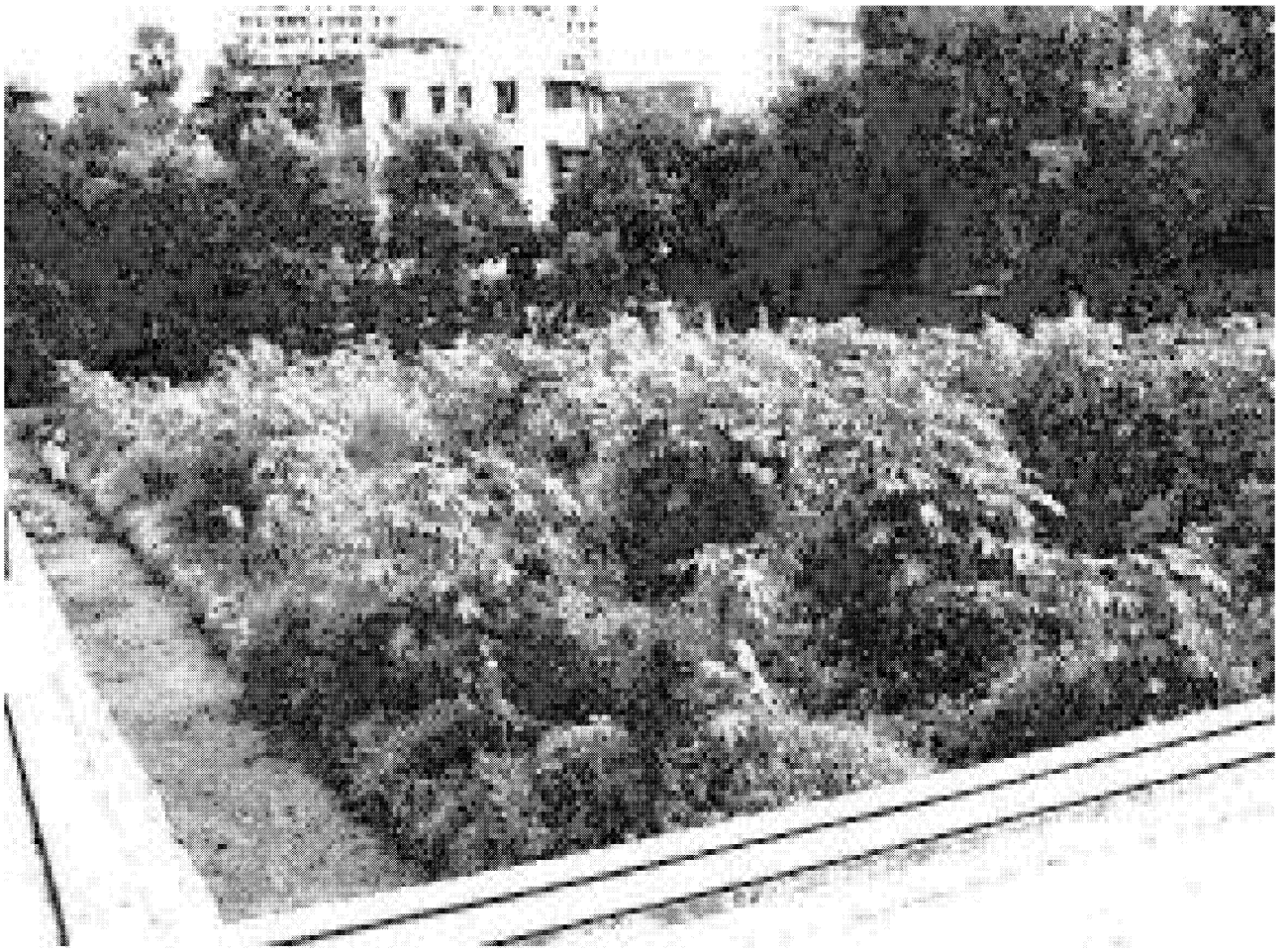


Figure 2: Fuly Commissioned SBT Bioreactor (Bombay Presidency Golf Club, Mumbai.)

Table 2: Specification of the bioreactor media (Pattanaik et al., 2003b)

Item	Details
Underdrain	Gravel - d_p = 25 mm, White Sand d_p = 2 mm,
Media*	Specific gravity- 2.62 BET specifica surface area- 23 m^2/g Cation Exchange capacity- 1.5 g/kg
Soil*	Sand: 67% Silt - 23%, Clay- 10% Specific gravity- 2.66 BET area- 33.6 m^2/g Cation Exchange capacity- 1.5 g/kg
Earthworm	*Phertima elongate*

d_p=Partical diameter. BET: Brunauer, Emmett &Teller (isotherm).
* - Particle size distribution is similar initially, but due to prolonged earthworm movement, it changes with time.

2 Experimental

2.1 Experimental Equipment

Schematic of the 1.6 m deep batch setup is shown in Fig 3. It consists of a reactor containing the media and a recycle tank. The reactor is made of cylindrical aluminum containers, mounted on a metal grid. Sampling ports were provided at every 0.25 m distance. The media in the bioreactor include a bottom layer of gravel (5 cm thick) followed by sand layer (2 cm thick) and finally the active formulated media (1.5 m thick).

A peristaltic pump is used to obtain desired flowrate. A distributor made of rubber tubes with holes ($\simeq$ 1 mm diameter) is used to obtain uniform distribution of the liquid over the surface of media. An overhead tank is used to store the liquid being recirculated from the recycle tank. Centrifugal pump is used to pass the liquid from recycle tank to the overhead tank.

2.2 Bioreactor Media

SBT bioreactors can be grouped in two broad categories - cultured and uncultured; based on the type of media used and the addition of worm culture.
Cultured bioreactor consists of a media housing an engineered ecology of soil, bioindicator plants, soil containing selected micro and macro-organisms such as geophagus earthworms. The media is formulated from variety of materials such as sand, silt, clay, etc and is bioprocesed before filling in the bioreactor. By addition of the earthworm culture, the rates of biological processes are enhanced to bring about the waste processing, as discussed in section 2.1. Bioconversion takes place via. bacterial processing of waste materials where geophagus worms serve as predator to select and regulate the bacterial action. Patents of Pattanaik et al. (2002, 2003a) cover details of culture media and additives used. *Uncultured bioreactors* contains media formulated from sand, silt and clay. (Table 2). No earthworm culture is added. So, the processing is carried out by the activity of selected microorganisms. Details of the media and underdrain used in the SBT bioreactors are given in Table 2. In this work uncultured bed refers to media specifications of Pattanaik et al. (2002, 2003a); cultured bed refers to reactors wherein media culture as specified by Pattanaik (2002, 2003a) is used.

2.3 Experimental Procedure

In a batch experiment, known volume of liquid substrate of interest (viz. sugar solution, glucose solution, sewage or wastewater or drinking water source) is taken in the recycle tank and circulated at a desired flow rate (50-400 L/m^{2}h) using a peristaltic pump. Usually a batch experiment runs

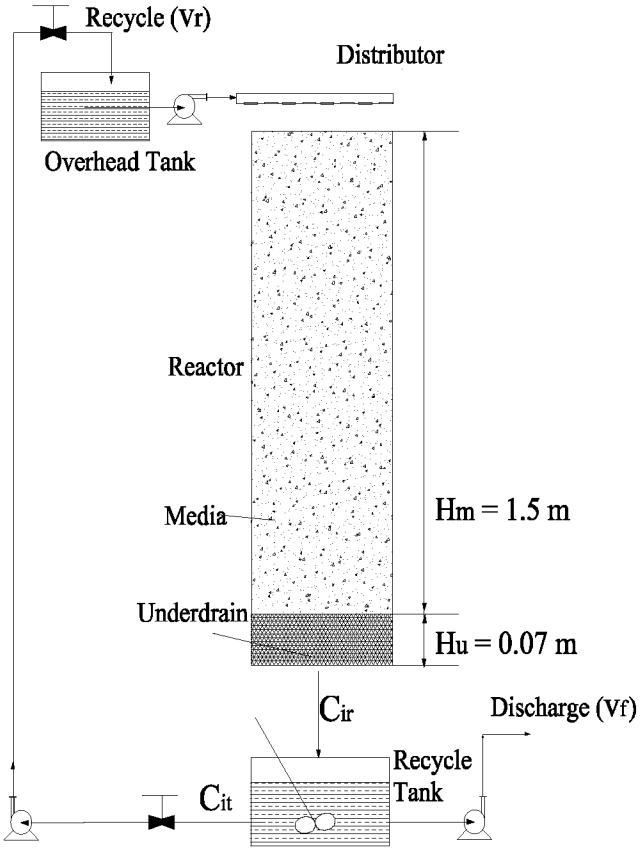


Figure 3: Schematic of Experimental Setup for 1.5 m deep Bioreactor.

for 4-6 hours and during this contacting time, solid liquid equilibrates. Sampling is done from the reactor exit and the recycle tank.

After a batch run, the bed is allowed to regenerate for about 16 h. During regeneration, the organics loaded on the media surface gets degreaded.

Sampling along the height of the bed was not possible, since the flow rates are very low, and hence the contact area between the sampling ports and the flowing fluid stream is very small. So, enough amount of sample could not be collected for analysis.

COD content of the sample was determined by using standard analytical procedure. (APHA et al., 1985). Experiments were performed for different combinations of bed volume, cultured/uncultured media, etc.; for different volumetric feed rate or initial COD content of the fluid. Average substrate removal rate is calculated as,

$$\overline{R_i} = \frac{(S_0 - S_f)V_l}{V_b t_b} \tag{1}$$

where, S_0 is the initial substrate concentration, S_f is final substrate concentration, V_l is volume of the process liquid, V_b is bioreactor volume and t_b is time of the batch run.

3 Computational Model of Soil Bioreactor

Fig 1 shows schematic of the processing of fluid through a porous packed bed bioreactor. To model the soil bioreactor using CFD, a lumped parameter approach is followed, treating the packed bed as anisoropic porous media. Thus, the flow through the bioreactor, liquid to solid mass transfer, and the kinetics of the major biological processes is defined with a series of sub-models such as

1. The momentum loss associated with the packing of the bed particles and the simulation of the anisotropy of the media and underdrain;
2. A surface reactions model to include adsorption, surface reactions and desorption;
3. A mass transfer model to represent the transfer of substrates between the circulating fluid and the bed particles, with consideration of non-equilibrium between the soild and the liquid;
4. Representation of the dispersion effects of the substarates in the fluid due to the presence of the porous particles;
5. A recycle tank model which gives the variation in substrate concentration at reactor inlet due to presence of recycle tank in circulation loop.

These sub-models translate the design/process information regarding the bioreactor into a CFD simulation that completly describes the process. Th model takes into account the convective and diffusive transport of solute and solvent and assumes that removal of substrate follows first order rate equation. For constant density system with low flow velocities, the equations describing conservation of mass and momentum are, (Bird et al., 2002)

$$\frac{\partial \rho}{\partial t} + \bigtriangledown \cdot (\rho \vec{v}) = 0 \tag{2}$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \bigtriangledown \cdot (\rho \vec{v} \vec{v}) = \vec{F} - \bigtriangledown p + \rho \vec{g} \tag{3}$$

where $\vec{F}$ is the momentum loss term describing the resistance to liquid flow offered by the porous media. For the present system, with low flow velocities through the bioreactor, Darcy's law is followed. (Viottoi et al., 2002).

$$\vec{F} = -\frac{\mu}{\alpha_j} \vec{v} \tag{4}$$

where α_j is the permeability of the medium in direction j. With diffusion flux given by Fick's law, the species conservation equation in terms of local species concentration in the fluid (C_i) is given as,

$$\frac{\partial (C_i)}{\partial t} + \bigtriangledown \cdot (\vec{v} C_i) = -\bigtriangledown \cdot (D_{i,m} \bigtriangledown C_i) + R_i + S_i \tag{5}$$

where, R_i is the rate of degradation of the substrate by biochemical reactions; and S_i is the addition of substrate by liquid-solid mass transfer, and from user defined sources.

During a batch operation, as the water is passed through the bioreactor, organic matter gets loaded on the media surface. This process consists of mass transfer of the substrate from liquid to the media surface followed by uptake; which may be by adsorption, ion-exchange, or by holdup inside the pores. Also, the products of the biochemical reaction such as $NO_3^- - N$, moves back to the liquid.

The substrate consumption rate (R_i) is a function of the rate of the biochemical reactions which mainly take place on the media surface. From Michaelis-Menten kinetics (Belly and Ollis, 1986),

$$R_i = \frac{K_m C_i}{K_{ms} + C_i} \tag{6}$$

For the case of SBT bioreactors, C_i being small, above equation reduces to $R_i = KC_i$, where $K = K_m / K_{ms}$. Also, the term $S_i = k_l a (C_i - C_i^*)$ represents the mass transfer of the substrate from liquid to the media surface. Using an uptake rate constant $k_a = k_l a$; we get $S_i = k_a (C_i - C_i^*)$.

Langmuir type isotherm is used to describe the distribution of species between solid and liquid. So the equilibrium substrate concentration loaded on media is

$$C_i^* = \frac{K_2 q_i}{K_1 - q_i} \tag{7}$$

where, q_i is the substrate loaded on the media surface. Various biochemical reactions taking place in the bioreactor are described. (Table 1). To study the performance of SBT bioractors, main reactions are oxidation of organic matter (Eqn 2.1), nitrification (Eqn 2.10 & 2.11) and de-nitrification (Eqn 2.12). Final forms of the rate processes for the substrates are written as given in Table 3.

Table 3: Rate equations for different substrates in bioreactor

Substrate	**Rate Process**	**Source Term** R_i & S_i
COD	Mass Transfer	(+) $k_{ac}(C_{COD} - C^*_{COD})$
COD	Oxidation	(-) $k_{qc}q_{COD}$
$NH_4^+ - N$	Mass Transfer	(+) $k_{an}(C_{NH_4^+} - C^*_{NH_4^+})$
$NH_4^+ - N$	Nitrification	(-) $k_{qn}q_{NH_4^+}$
$NO_3^- - N$	Nitrification	(+) $k_{qn}q_{NH_4^+}$
Oxygen	Mass Transfer (Aeration)	(+) $k_{a2}(C^*_{o_2} - C_{o_2})$
Oxygen	Oxidation Reactions	(-) $Y_1 k_{qc} q_{COD}$
Oxygen	Nitrification	(-) $Y_2 k_{qn} q_{NH_4^+}$

$$C^*_{COD} = \frac{K_{c2}\ q_{COD}}{(K_{c1} - q_{COD})} \quad \& \quad C^*_{NH_4^+} = \frac{K_{n2}\ q_{NH_4^+}}{(K_{n1} - q_{NH_4^+})}$$

Table 4: Properties and parameter values for CFD simulation of bio-reactor

Description	**Symbol**	**Units**	**Value**	**Source**
Dynamic viscosity of the liquid phase	μ_l	kg/ms	0.001	Viotti et al., 2002
Density of the liquid phase	ρ_l	kg/m^3	998.2	Viotti et al., 2002
Glucose diffusivity in the liquid phase	D_G	m^2/s	6.7x10^{-10}	Viotti et al., 2002
$NH_4^+ - N$ diffusivity in liquid phase	D_{NH_4}	m^2/s	1.7x10^{-10}	Viotti et al., 2002
Oxygen diffusivity in liquid phase	D_{O_2}	m^2/s	2.3x10^{-9}	Viotti et al., 2002
Langmuir isotherm parameters	K_{c1}	g/l	6	Pattanaik, 2000
for COD	K_{c2}	g/L	0.3	
Langmuir isotherm parameters	K_{n1}	g/l	1.55	Pattanaik, 2000
for $NH_4^+ - N$	K_{n2}	g/L	0.1	
COD Uptake rate constant	k_{ac}	h^{-1}	1 - 3	Pattanaik, 2000
$NH_4^+ - N$ Uptake rate constant	k_{an}	h^{-1}	6-11	Pattanaik, 2000
COD degradation rate constant	k_c	h^{-1}	0.04-0.05	Pattanaik, 2000
Nitrification rate constant	k_n	h^{-1}	1.1-1.6	Pattanaik, 2000

Presence of recycle tank in the circulation loop for a batch process introduces time lag for variation of substrate concentration at reactor inlet with time for all the species. This variation of substrate conc. in recycle tank, C_{it} is given as

$$\tau_h \frac{dC_{it}}{dt} = C_{ir}(t) - C_{it}(t) \tag{8}$$

where, $\tau_h = \frac{(V_l - V_d)}{v_r}$ is recycle tank holding time; C_{ir} is the concentration at reactor outlet. concentration in the recycle tank (or reactor inlet).

CFD simulation involves selection of suitable physical models and standard functions defined in FLUENT to represent the system under consideration. For simulation of bioreactor model, the standard models provided in FLUENT solver were not sufficient to describe the system. Hence, user-defined functions (UDF) are used to customize the solver as per requirement to model the bioreactor. UDFs are used to define variation of porosity along the bed dimensions; permeability (viscous resistance) for the media and under-drain; rate terms for the species; and to model the time variation of species concentration entering the bioreactor due to presence of recycle tank.

Two dimensional (2D) grid was generated for different cases of bioreactor configurations as given in Table 5, using *Gambit* and exported to *Fluent*. The model is simulated for different laboratory and field scale devices. Three cases are considered viz. 30 cm and 1.75 m deep cylindrical beds and commercial facilities. Table 4 gives the properties and parameter values used for CFD simulation of bioreactor.

Table 5: Dimensions for bioreactors used in experiments and simulations

Parameter	A	B	C	D
Depth of Media, H_m (m)	0.26	1.5	1.5	0.54
Depth of underdrain, H_u (m)	0.04	0.1	0.3	0.1
Diameter of soil bed, D_b (m)	0.3	0.3	-	0.3
Surface area of soil bed, A_b (m^2)	0.07	0.07	-	0.07
Volume of bed, V_b (m^3)	0.016	0.113	-	0.042

A, B & D - Laboratory beds, C - Commercial facility having tetrahedral cross-section, base = 11.2 m, top surface width=6 m (Fig. 4)

4 Results and Discussion

4.1 Permeability of media

Flow characteristics of soil bed bioreactors differ in axial and radial directions. This results from the presence of micro channels and macro channels formed due to the burrowing movement of the macro-organisms such as earthworms, presence of root zones, etc. which form channels mainly in vertical direction. Permeability values for some materials are given in Table 6.

Simulations were performed for a large scale SBT bioreactor (Table 5-C) with ratio of $\frac{\alpha_a}{\alpha_r} = 1 - 10$. Results are shown in Fig 4. Results with $\frac{\alpha_a}{\alpha_r} = 1$, i.e. for isotropic media, are given in Fig. 4(A) in the form of contours of velocity magnitude. Velocity magnitude remains uniform over a larger portion of the bed cross-section, which is an indication of uniform liquid distribution. As the permeability ratio is increased to $\frac{\alpha_a}{\alpha_r} = 10$, fluid moves mainly in axial direction, as seen from Fig. 4(B) and 4(C). Thus channeling is observed. If the permeability ratio is even higher, say $\frac{\alpha_a}{\alpha_r} = 100$, increased amount of channeling would result in stagnent regions.

Experimental and practical field scale observations indicate that the ratio, $\frac{Pe_r}{Pe_a}$ is roughly equal to the ratio $\frac{\alpha_a}{\alpha_r}$. The results from Baten et al. (2001) for flow through structured packings indicate that the ratio, $\frac{Pe_r}{Pe_a} \simeq 10$. Thus, estimates for the magnitudes of radial permeability can be made, from results available from RTD measurements and from laboratory study of permeability in axial direction. These estimates will be useful for CFD simulations of such systems.

For SBT bioreactors, ratio of axial to radial permeability,(α_a/α_r) from available measurements, is approximately 2. (Table 6). In cultured bioreactors, due to presence of microchannels, the ratio can be in the range of 2-10 or even higher.

Table 6: Permeability values of some Geologic Materials

Material	K_h (m/h)	α (m^2)	Type of Measurement	Reference
Gravel, Coarse	6.25	6.375 x 10^{-7}	R	Todd, 1980
Sand, Medium	0.50	5.1 x 10^{-8}	R	Todd, 1980
Sand, Fine	0.104	1.06 x 10^{-8}	R	Todd, 1980
Clay	8.33e-5	8.5 x 10^{-7}	H	Todd, 1980
Silt	0.0034	3.41 x 10^{-10}	H	Todd, 1980
Media	0.067	6.8 x 10^{-9}	H	Pattanaik, 2000
Media	0.034	3.47 x 10^{-9}	V	Pattanaik, 2000

$\alpha = \frac{\mu}{\rho g} K_h$ where, K_h - Hydraulic Conductivity, α - Permeability, R - Repacked Sample, H - Horizontal Hydraulic Conductivity , V - Vertical Hydraulic Conductivity.

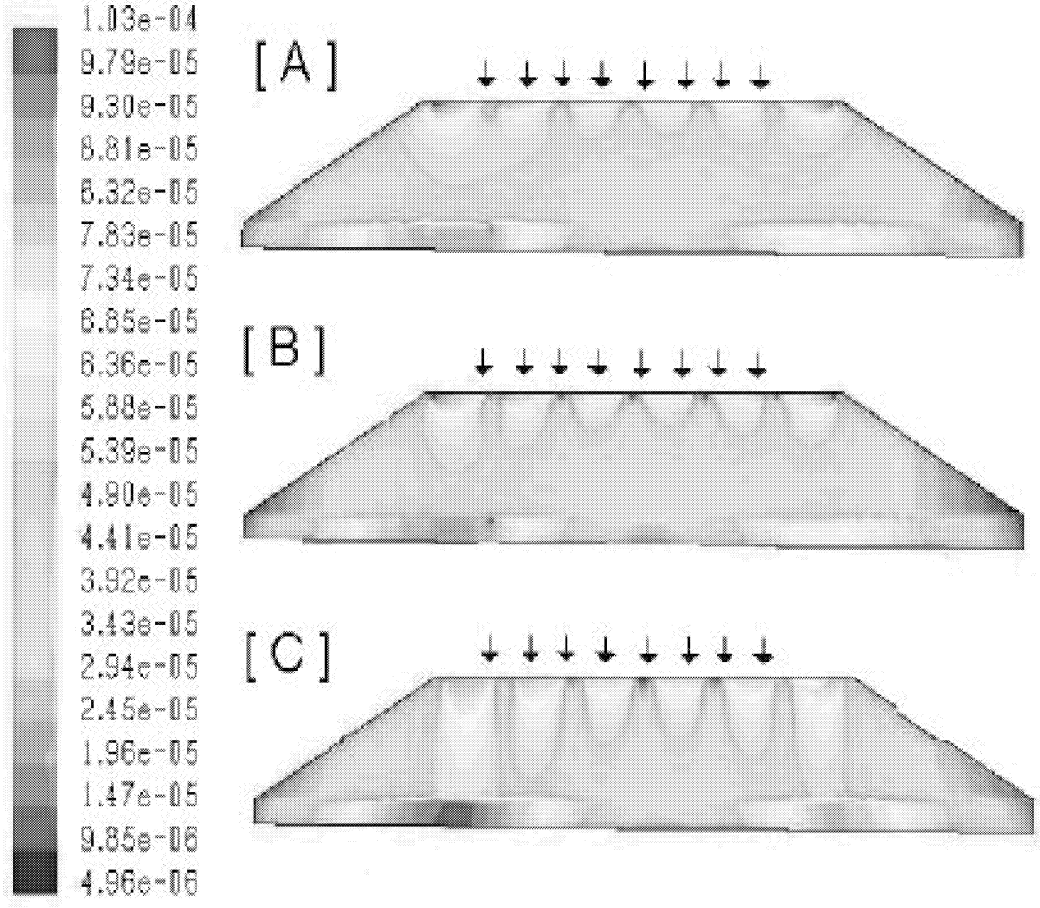


Figure 4: Effect of permeability variation on velocity profile (m/s). Dimensions of the tetrahedral bioreactor crosssection are: base width = 11.2 m, Height of media layer H_m = 1.5m, Height of Underdrain H_u = 0.3 m. v_r = 0.15 m^3/m^2h. (A) Isotropic media, $\alpha_a = \alpha_r = 1.25x10^{-10}m^2$; (B) Anisotropic media, α_a = 5x10^{-10} m^2, α_{rad} = 1.25x10^{-10} m^2; (C) Anisotropic media, α_a = 1.25x$10^{-9}m^2$, α_r = 1.25x10^{-10} m^2

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4.2 Feed Distribution Arrangement

For bioreactors with large surface area, uniform distribution of the feed over the surface is necessary to obtain good contact of fluid with the media; and hence for better utilization of the reactor. Fig. 5 shows the velocity profiles for simulations with different feed arrangements for a commercial bioreactor (Table 5-C).

In first case; (Fig 5a), fluid enters the bed only from top surface as indicated by the arrows. Here, some regions at the bottom of the bioreactor show zero velocity magnitude. This indicates that fluid has not distributed in entire bed volume.

In second case; (Fig 5b), 70 % water enters from top and 30% water is fed from the slopes of the bed as indicated by arrows. Here, uniform velocity contours are observed over a larger protion of the bed cross-section. This suggest uniform fluid distribution.

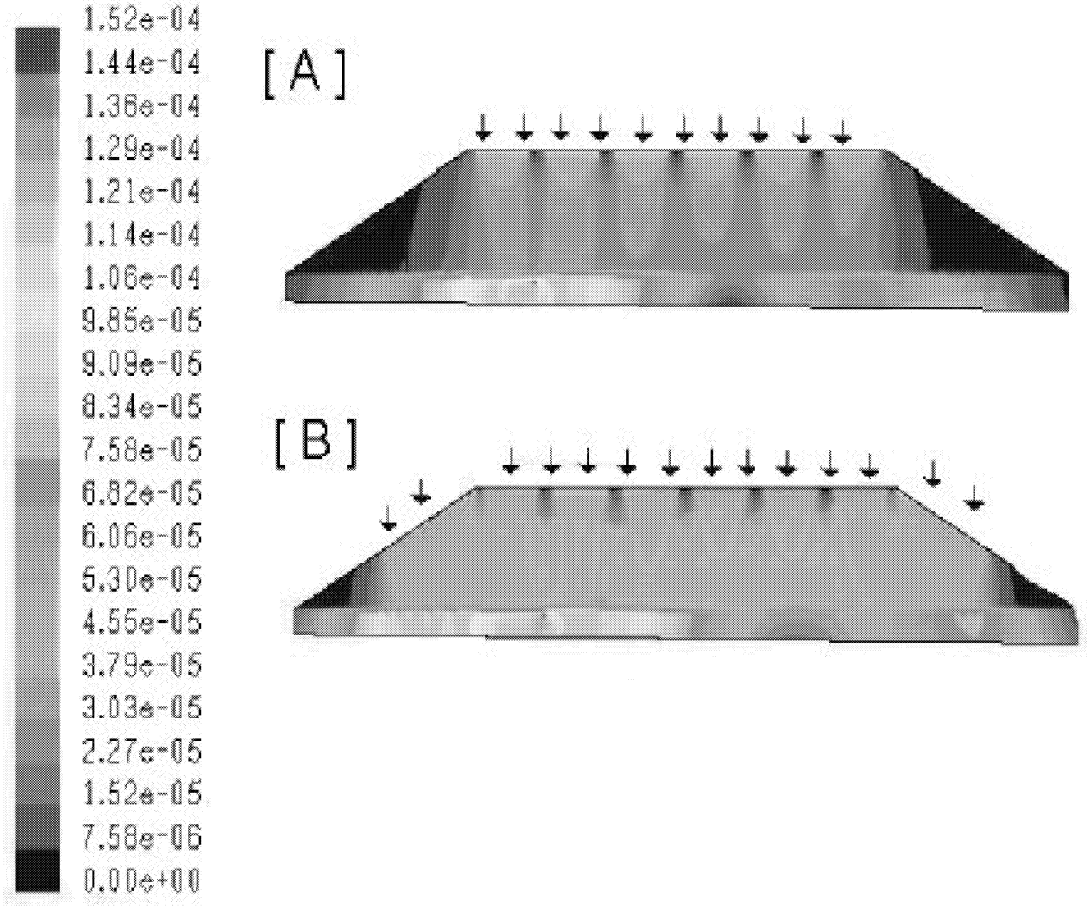


Figure 5: Effect of feed distribution arrangement on velocity profile. Velocity variation in the range 10^{-6}-10^{-4} m/s Superficial flow velocity, v_r=0.15 m^3/m^2h, α_a = 7x$10^{-10}m^2$, α_r = 2x10^{-10} m^2. (A) Water entering from top only. (B) 70 % of water entering from top, 30 % water entering from slopes.

4.3 Flow velocity

Fig. 6 shows the simulation results for substrate removal with different fluid velocities (v_r). As the fluid velocity is increased within the operating range of bioreactors, uptake of COD and ammoniacal-nitrogen increases. These predictions are similar to the trend observed with laboratory and field soil filters. The results are summarized in Table 7.

Uptake of solute during batch process depends on the fluid-solid contact and the residence time of fluid in the bioreactor. With increased superficial fluid velocity, dynamic holdup (V_d) also increases, increasing the fluid solid contact. With this, removal of substrate also increases.

Table 7: CFD Simulation Results for substrate removal: Variation with flow velocity. System paramters : V_b = 113 L, V_l = 25 L, t_b = 6 h. (Fig. 6)

Flow Velocity	**Dynamic Holdup**	**COD Removal**			$NH_4^+ - N$ **Removal**		
v_r (L/m^{2}h)	V_d (L)	Initial (mg/L)	Final (mg/L)	$\overline{R}_{COD}$ (mg/L h)	Initial (mg/L)	Final (mg/L)	$\overline{R}_{NH_4^+-N}$ (mg/L h)
84.86	6	500	225	15.21	20	3.8	1.195
169.7	7	500	120	21.02	20	1.9	1.335
254.5	8.5	500	61	24.28	20	0.6	1.431
339.5	10	500	27	26.16	20	0.25	1.456

Removal Rate, $\overline{R_i} = \frac{(S_0 - S_f)V_l}{V_b t_b}$. t_b = 4 h for all cases.

4.4 Species Transport and Kinetics

Comparison of CFD simulations for batch experiments together with known kinetic parameters indicate that CFD model captures the features of the process very well.

Fig. 7 - 10 shows plots for COD and $NH_4^+ - N$ concentration of fluid with time for cultured bioreactors. For cultured media, COD uptake rate constant, k_{ac} is observed to be 2.5-2.7 h^{-1}; while $NH_4^+ - N$ uptake rate constant, k_{an} is observed to be 10.2-11 h^{-1}. Thus for cultured bed, high rates of substrate removal are obtained. The results are summarised in Table 8. It can be seen that main variables deciding the uptake rates are flow velocities and initial substrate concentrations.

Fig. 11 & 12 shows plots for COD concentration of fluid with time for uncultured bioreactors of 0.3, 0.6 and 1.5 m deep. As the CFD model uses Langmuir isotherm parameters predicted for cultured bioreactors, the model shows deviation from the experimental data. The results are summarised in Table 9.

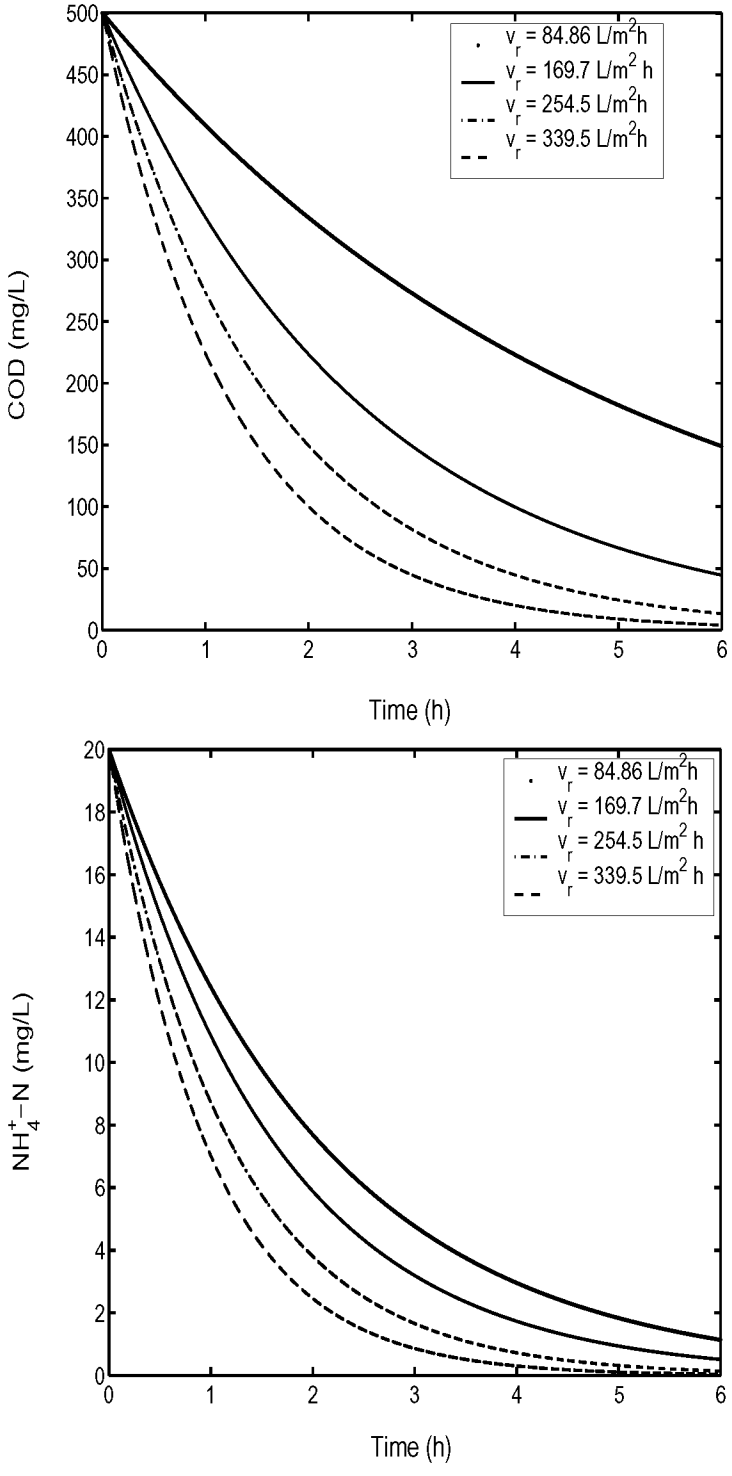


Figure 6: COD and $NH_4^+ - N$ Concentration of fluid: variation with fluid velocity for cultured bioreactors(V_b =113 L, V_l=30 L, k_{ac}=1.5 h^{-1}, k_c=0.05 h^{-1}, k_{an}=11 h^{-1}, k_n=1.5 h^{-1}, α_a = 7x$10^{-10} m^2$, α_r = 2x10^{-10} m^2)

Table 8: Comparison of results of CFD simulation and Experimental data for Cultured Bioreactors

Run No.		BB15	BB16	BB17	BB20
V_b (L)		13	13	13	13
V_l (L)		30	30	30	10
t_b(h)		5.5	5.0	5.0	7
v_r (L/h)		32.4	36	36.6	6
COD Removal					
Experimental	Initial (mg/L)	197.37	227.1	81	212
	Final (mg/L)	51	59	26	88
	$\overline{R}_{COD}$ (mg/Lh)	61.41	75.58	25.38	15.89
CFD Simulation	Initial (mg/L)	197.37	227.1	81	212
	Final (mg/L)	42	51	24	88
	$\overline{R}_{COD}$ (mg/Lh)	65.19	81.28	26.31	15.89
$NH_4^+ - N$ Removal					
Experimental	Initial (mg/L)	5.27	4.02	7.31	9.8
	Final (mg/L)	0.29	0.36	0.68	0.36
	$\overline{R}_{NH_4^+-N}$ (mg/Lh)	2.08	1.69	3.06	1.036
CFD Simulation	Initial (mg/L)	5.27	4.02	7.31	9.8
	Final (mg/L)	0.17	0.1	0.5	0.3
	$\overline{R}_{NH_4^+-N}$ (mg/Lh)	2.14	1.81	3.14	1.044

$A_b = 0.067$ m^2, Average Removal Rate, $\overline{R_i} = \frac{(S_0 - S_f)V_l}{V_b t_b}$.

Table 9: Comparison of results of CFD simulation and Experimental data for Uncultured Bioreactor

Run No.		M1	MB02	MB03	MB04
V_b (L)		16	40	113	113
V_l (L)		15	15	20	27
t_b(h)		4	4	3	4
v_r (L/h)		18	18	15	15
COD Removal					
Experimental	Initial (mg/L)	430	323	501	500
	Final (mg/L)	228	145	143	230
	$\overline{R}_{COD}$ (mg/Lh)	47.34	16.68	21.12	12.66
CFD Simulation	Initial (mg/L)	430	323	501	500
	Final (mg/L)	150	137	30	140
	$\overline{R}_{COD}$ (mg/Lh)	65.625	17.44	27.79	21.5

$A_b = 0.07$ m^2, Average Removal Rate, $\overline{R_i} = \frac{(S_0 - S_f)V_l}{V_b t_b}$.

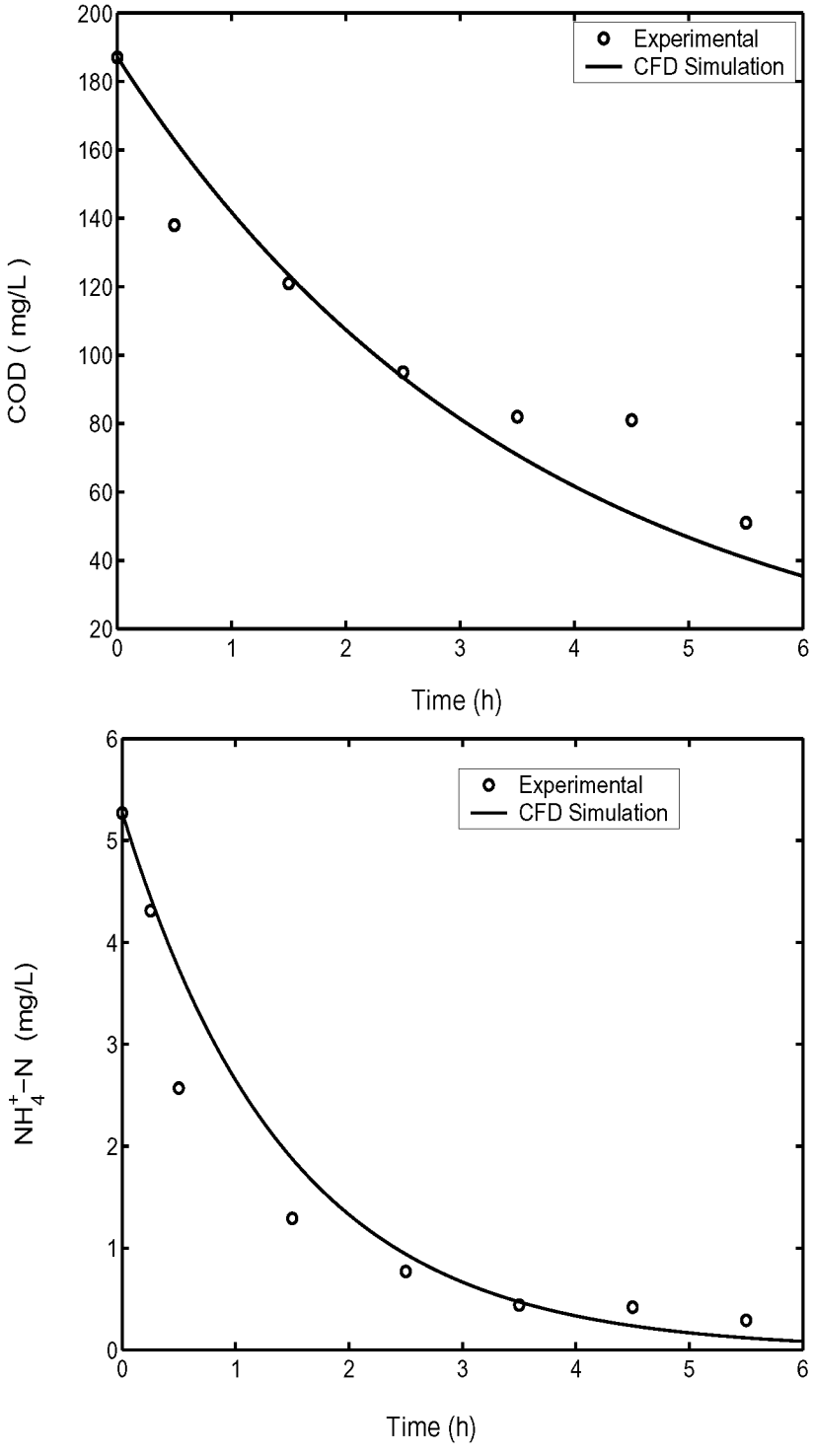


Figure 7: COD and $NH_4^+ - N$ Concentration of fluid with time: comparison with experimental results for cultured bioreactor.(BB15)(V_b =13 L, V_l=30 L, v_r=32.4 L/h, k_{ac}=2.4 h^{-1}, k_c=0.05 h^{-1}, k_{an}=10.4 h^{-1}, k_n=1.5 h^{-1}, α_a = 7x$10^{-10}m^2$, α_r = 2x10^{-10} m^2).

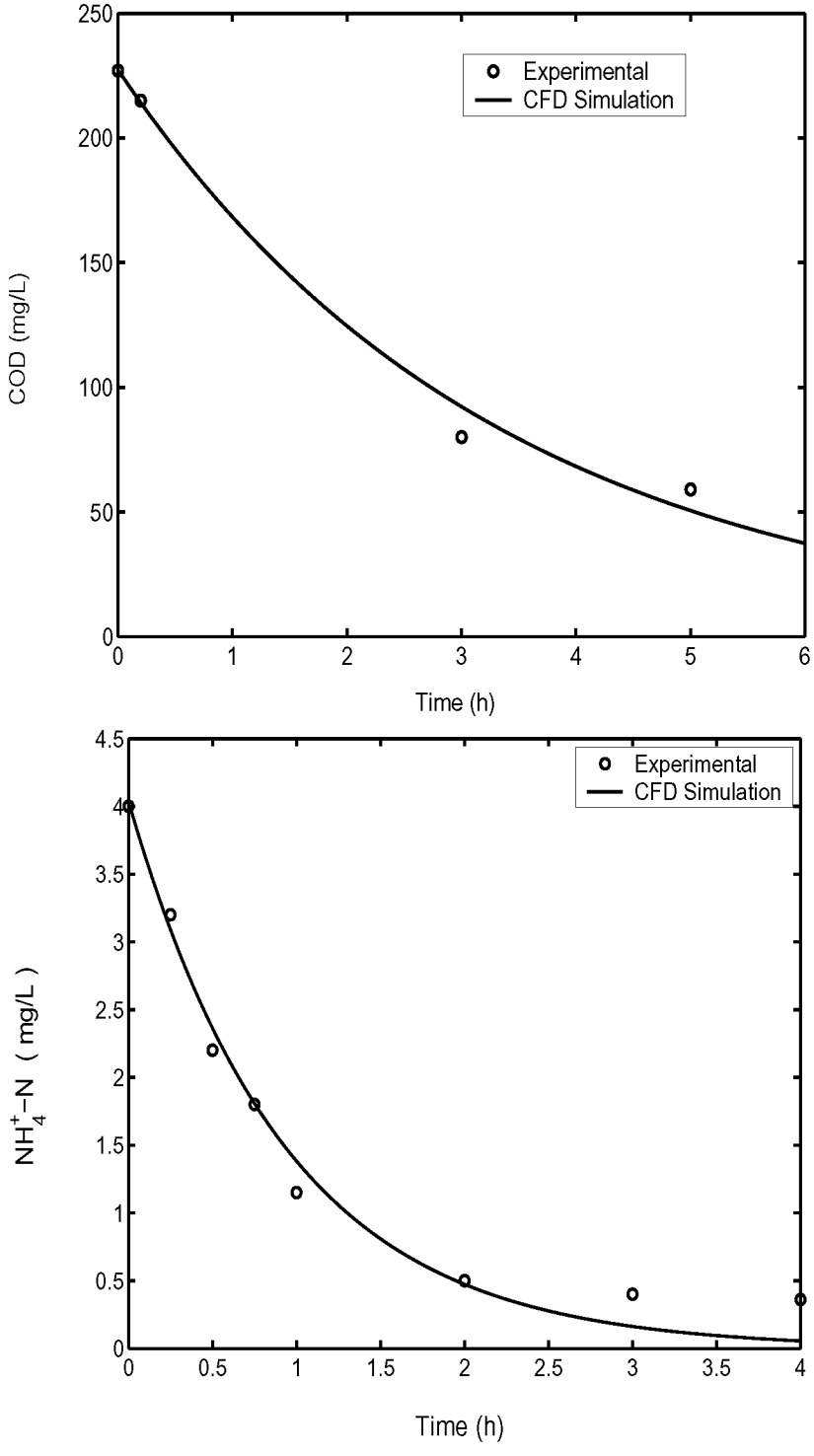


Figure 8: COD and $NH_4^+ - N$ Concentration of fluid with time: comparison with experimental results for cultured bioreactor.(BB16) (V_b =13 L, V_l=30 L, v_r=36 L/h, k_{ac}=2.45 h^{-1}, k_c=0.05 h^{-1}, k_{an}=10.6 h^{-1}, k_n=1.5 h^{-1}, $\alpha_a = 7\text{x}10^{-10} m^2$, $\alpha_r = 2\text{x}10^{-10}$ m^2.)

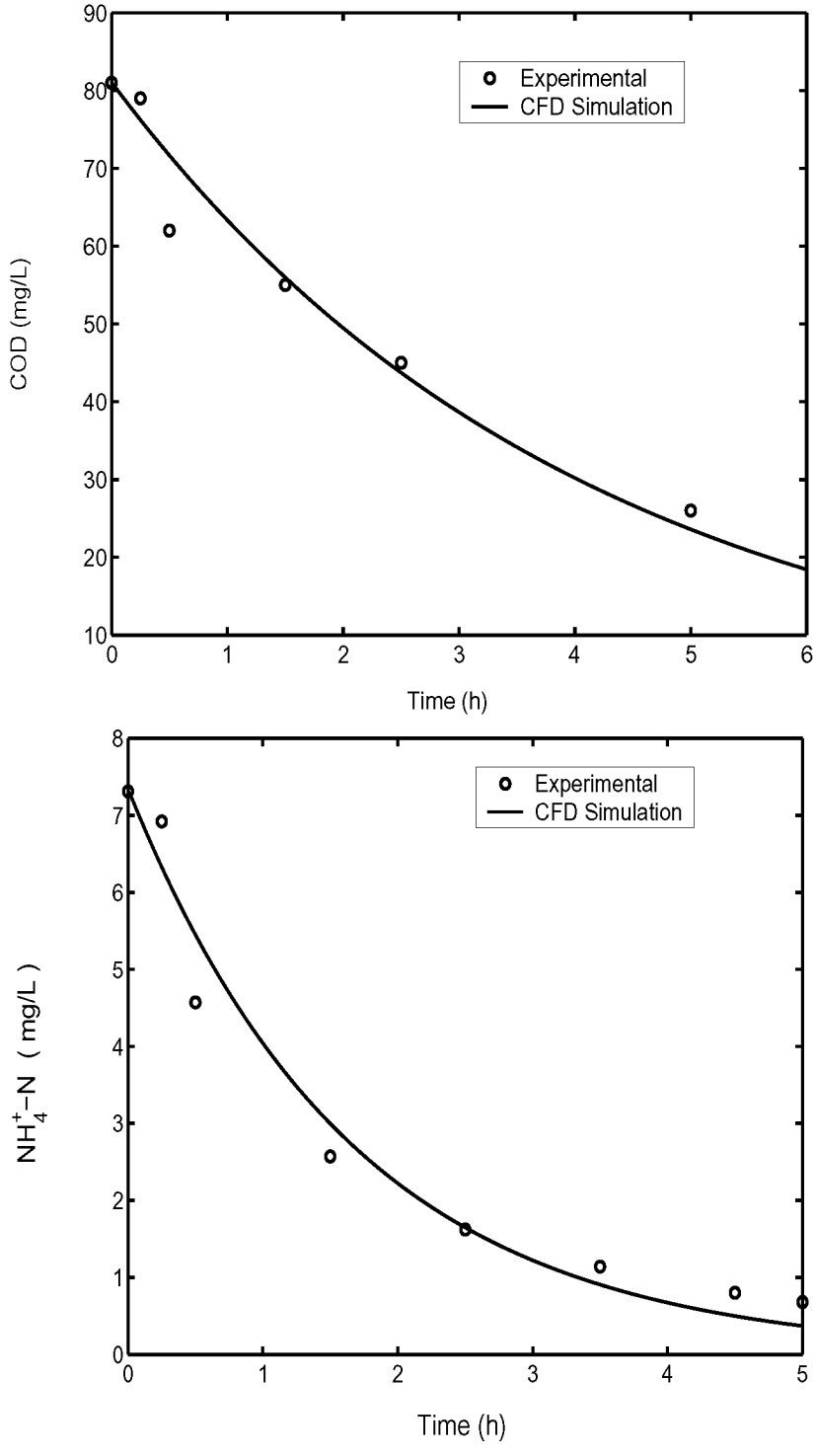


Figure 9: COD and $NH_4^+ - N$ Concentration of fluid with time: comparison with experimental results for cultured bioreactor.(BB17) (V_b = 13 L, V_l = 30 L, v_r = 36 L/h, k_{ac} = 2.45 h^{-1}, k_c = 0.05 h^{-1}, k_{an} = 11 h^{-1}, k_n = 1.5 h^{-1}, α_a = 7x$10^{-10}m^2$, α_r = 2x10^{-10} m^2)

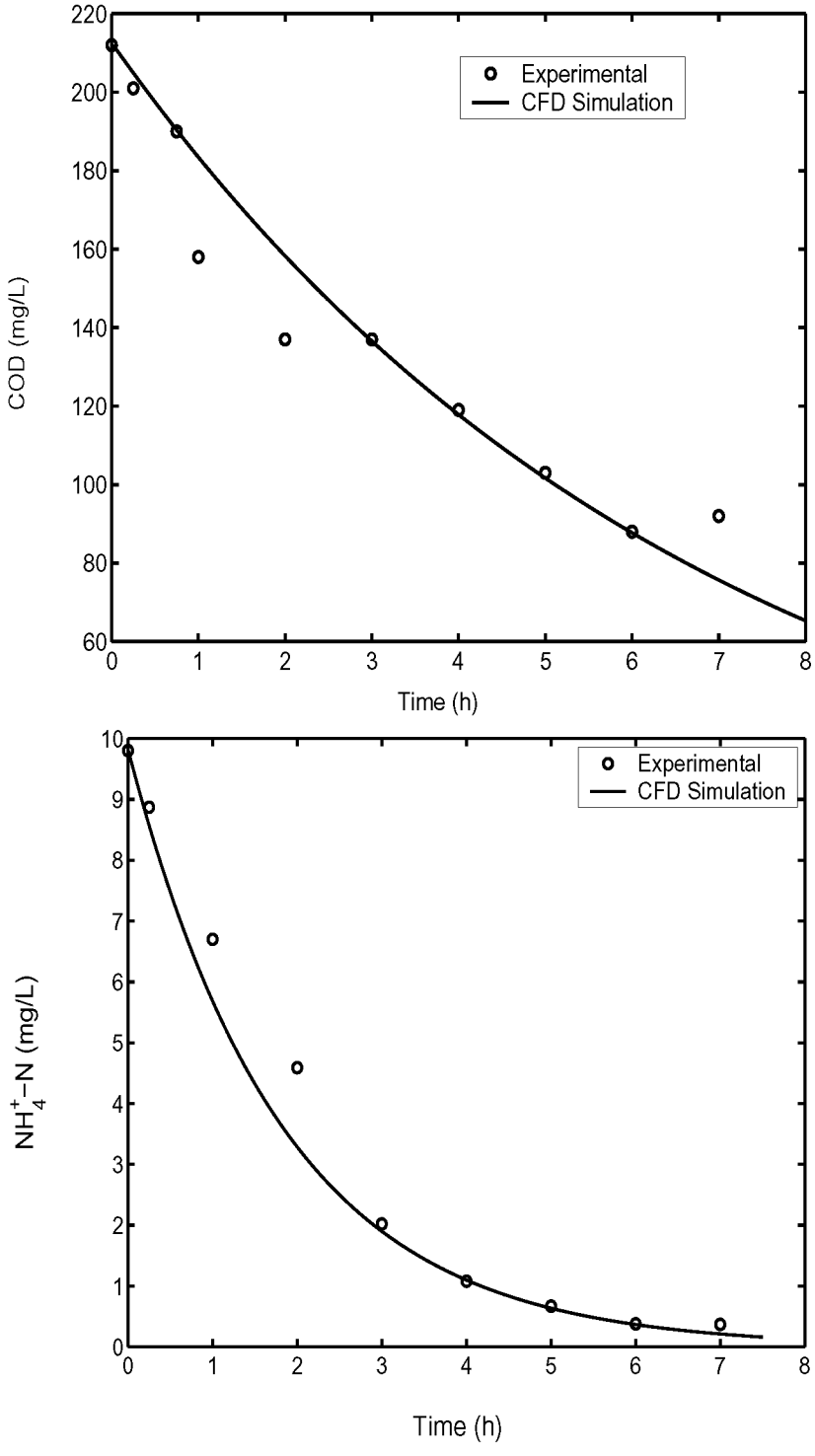
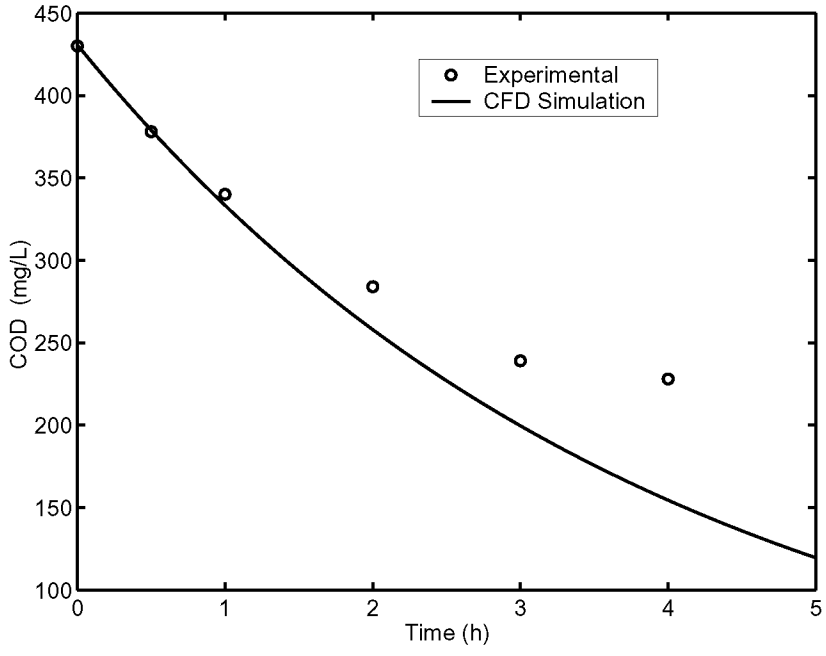
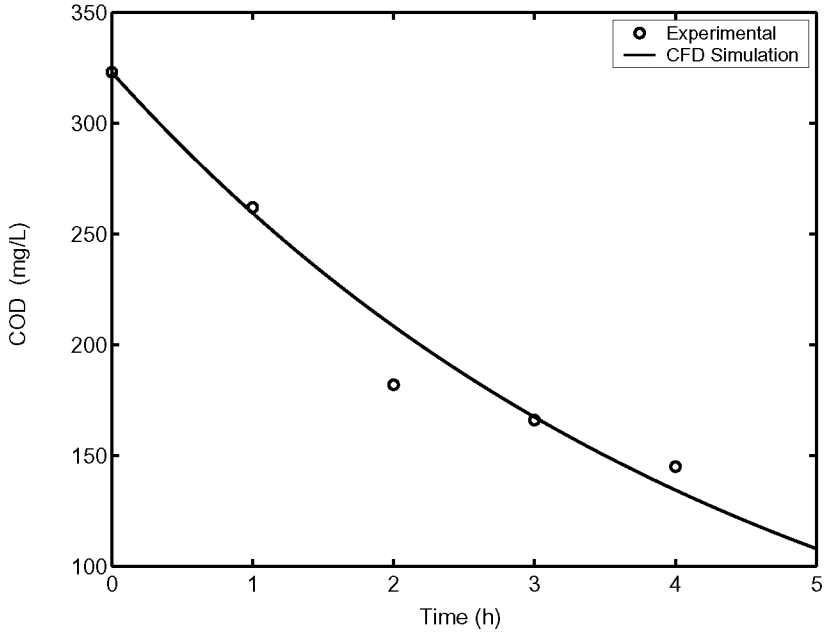


Figure 10: COD and $NH_4^+ - N$ Concentration of fluid with time: comparison with experimental results for cultured bioreactor.(BB20) ($V_b = 13$ L, $V_l = 10$ L, $v_r = 6$ L/h, $k_{ac} = 2.2$ h^{-1}, $k_c = 0.05$ h^{-1}, $k_{an} = 10.4$ h^{-1}, $k_n = 1.26$ h^{-1}, $\alpha_a = 7\text{x}10^{-10} m^2$, $\alpha_r = 2\text{x}10^{-10}$ m^2)

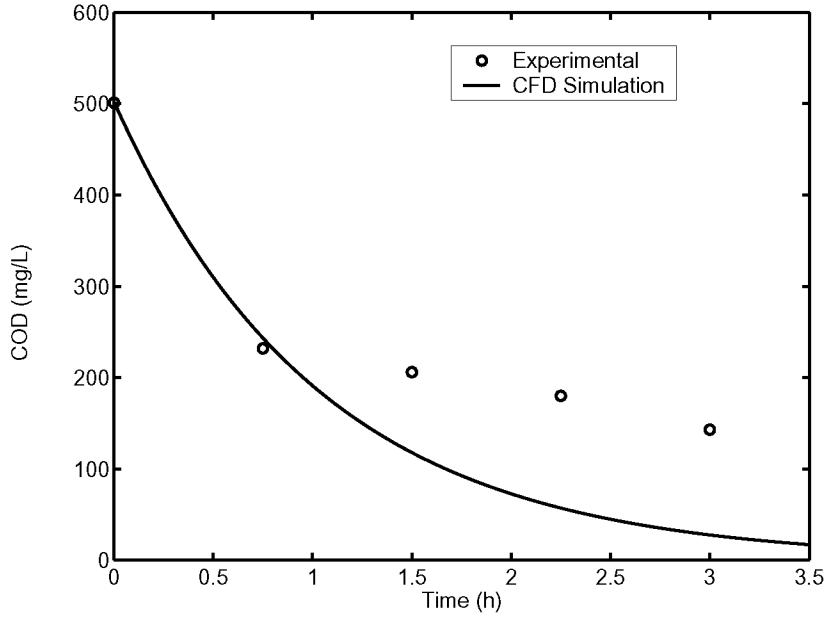


(a) M1

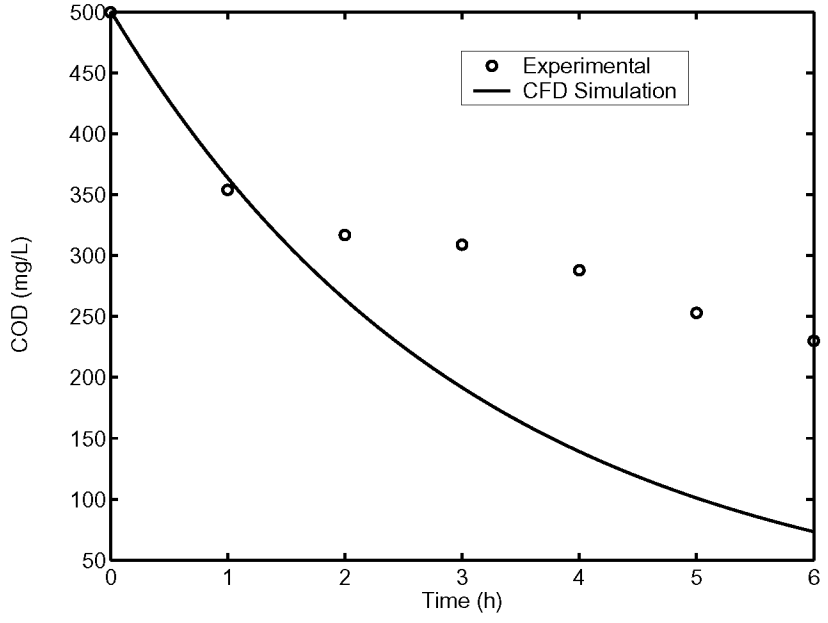


(b) MB02

Figure 11: COD Concentration of dextrose solution with time: comparison with experimental results for 0.3 m and 0.6 m deep uncultured Bioreactors. (A) V_b = 16 L, V_l = 18 L, v_r = 15 L/h, k_{ac} =1.3 h^{-1}, k_c = 0.04 h^{-1}.(B) V_b = 40 L, V_l = 15 L, v_r = 18 L/h, k_{ac} = 0.95 h^{-1}, k_c = 0.04 h^{-1}, α_a = 7x10$^{-11}m^2$, α_r = 2x10^{-11} m^2.



(a) MB03



(b) MB04

Figure 12: COD Concentration of dextrose solution with time: comparison with experimental results for 1.6 m deep uncultured bioreactor. (C) V_b = 113 , V_l = 20 L, v_r = 15 L/h, k_{ac} = 0.95 h^{-1}, k_c = 0.04 h^{-1}. (D) V_b = 113 L, V_l = 25 L, v_r = 15 L/h, k_{ac} = 0.8 h^{-1}, k_c=0.04 h^{-1}, α_a = 7x10$^{-11}m^2$, α_r = 2x10^{-11} m^2.

5 Conclusions

The work presented leads to the following conclusions,

1. CFD for modelling flow and reaction through porous SBT bioreactor is a novel way of understanding such bioreactors.

2. CFD model of SBT bioreactor is based on basic conservation principles and is scale dependent. It captures the local effects in the system; reducing the scale-up problems. Thus, performance of large scale systems can be estimated by making use of permeability (α) and rate parameters; determined from simpler laboratory and field scale measurements. So CFD provides a powerful tool for scale-up.

Nomenclature

Symbol	**Interpretation**	**Units**
A_b	Cross sectional area of laboratory bioreactor	m^2
C_i	Molar concentration of species i	$kmol/m^3$
C_{COD}	COD concentration	mg/L
$C_{NO_3^-}$	NO_3^- concentration	mg/L
$C_{NH_4^+}$	NH_4^+ concentration	mg/L
$C^*_{NH_4^+}$	Equilibrium conc. of NH_4^+	g/L
C^*_{COD}	Equilibrium conc. of COD	g/L
C_{ir}	Concentration of species i at reactor outlet	mg/L
C_{it}	Concentration of species i in recycle tank	mg/L
D_b	Diameter of soil bed	m
D_G	Glucose diffusivity in the liquid phase	m^2/s
D_{NH_4}	Ammonia-nitrogen diffusivity in liquid phase	m^2/s
D_{O_2}	Oxygen diffusivity in liquid phase	m^2/s
$D_{i,m}$	Diffusivity of species *'i'* in the mixture	m^2/s
H_b	Total depth of bioreactor	m
H_m	Depth of media	m
H_u	Depth of underdrain	m
K_h	Hydraulic conductivity	m/h
K_{c1}, K_{c2}	Langmuir isotherm parameters for COD	kg/m^3
K_{n1}, K_{n2}	Langmuir isotherm parameters for $NH_4^+ - N$	kg/m^3
k_{ac}	COD Uptake rate constant	h^{-1}
k_{an}	$NH_4^+ - N$ Uptake rate constant	h^{-1}
k_n	Nitrification rate constant	h^{-1}
K_m	Maximum rate coefficient of substrate	kg/kg
K_{ms}	Half saturation constant	kg/m^3
q_{COD}	COD loaded on media surface	kg/m^3 of solid
$q_{NH_4^+}$	$NH_4^+ - N$ loaded on media surface	kg/m^3 of solid
p	Static pressure	pa
Pe	Peclet number (dimensionless)$(=\frac{uL}{D})$	
R_i	Rate equation for species *'i'*	kmol/ m^3 h
t	Time	h
t_b	Batch time	h
V_b	Filter Bed volume	m^3
V_l	Volume of Process liquid	m^3
v_r	Recycle flow rate	m^3/m^2h
Y_1, Y_2	Stoichiometric factors for oxidation of COD and $NH_4^+ - N$ respectively	kg/kg

Greek letters

α	Fraction of macro channel in bed volume	
α	Permeability	m^2
α_a	Axial permeability	m^2
α_r	Radial permeability	m^2
β	Fraction of micro channel in bed volume	
ϵ_d	Dynamic hold up fraction of total bed volume	
ϵ	Porosity of Packed Bed [Soil Bed]	
ρ	Density of liquid	kg/m^3
τ	Space time	h
θ	Dimensionless time	
μ	Viscosity of liquid	kg/m.s
τ_h	Recycle tank holding time	h

Abbreviations

BOD	Biological Oxygen Demand
CFD	Computational Fluid Dynamics
COD	Chemical Oxygen Demand
DO	Dissolved Oxygen
MCM	Mixed Cell Model
RTD	Residence Time Distribution
SBT	Soil Biotechnology
SBR	Soil Bioreactor
TCDM	Two Channel Dispersion Model
UDF	User Defined Function

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