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# MATHEMATICAL MODELLING OF A FLUIDISED BED BIOREACTOR

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## ABSTRACT

*A mathematical model of a fluidised bed bioreactor was presented and analysed. The model is for zero order intrinsic reaction kinetics. Modified effectiveness factor and modified Thiele modulus were developed to quantify intrabiofilm mass transfer resistances. The modified effectiveness factor is incorporated in overall FBB model which is analytically solvable and thus, is a convenient tool for system analysis and design.*

*From a kinetic model of the biofilm it was found that for zero order kinetics, a situation where transition occurs from full to partial substrate penetration of the biofilm is determined by the value of modified Thiele modulus* $\phi_{om}$. *For* $\phi_{om} < 1.15$, *the whole biofilm is active and intrinsic zero order kinetics are observed. When* $\phi_{om} > 1.15$, *the inner portion of the biofilm is inactive and the observed reaction rate is proportional to the value of* $S_b^{0.55}$.

*The simplified model of a bioreactor was also presented and analysed. It was established that this model was also capable of describing the observed bioreactor kinetic behaviour with the accuracy satisfactory for industrial practice. Thus, the simplified model can provide a rational basis for design and optimization of a bioreactor. The optimal values of the two most important parameters for efficient performance of the bioreactor, viz. biofilm thickness and media size, that maximize the substrate conversion rate can be determined from that model.*

## INTRODUCTION

Biological fixed films exhibit properties that make them preferable to suspended-cell systems for many continuous bioprocess applications. These properties include the high cell concentrations, enhanced cell retention

due to cell immobilisation and an increased resistance to the detriment effects of toxic shock loadings [1,2]

A fluidised bed bioreactor (FBB) has received increasing interest and wide utilisation in both fermentation processes and wastewater treatment [3,4]. The FBB outperforms other bioreactor configurations such as activated sludge system and packed-bed (or trickling-filter) bioreactor [1,4,5]. The superior performance of the FBB stems from the high biomass concentration (up to 30 - 40 kg/m$^3$) that can be achieved in the bioreactor due to immobilisation of cells onto or into the solid particles. Once fluidised, the particles provide a large surface area for biofilm formation and growth. Each support eventually becomes covered with biofilm and the vast available growth support surface afforded by the media results in a biomass concentration approximately an order of magnitude greater than that maintained in a suspended growth system [3,6].

The use of biomass support allows the replenishment of the fluidised bed without interrupting the operation and thus, maintains high microbial activity. Consequently, the limit on the operating liquid flow rates imposed by the microbial maximum specific growth rate is eliminated due to the decoupling of the residence time of the liquid phase and of the growth of microbial cells.

In this work a kinetic model of a fluidised bed bioreactor is presented and analyzed. The model was derived through the principles of solid-liquid fluidisation and heterogeneous catalysis. A simplified model of a bioreactor was also presented and validated.

## MATHEMATICAL MODEL OF A FBB

The model presented below was derived under assumption that the substrate conversion, that follows intrinsic zero-order kinetic, is limited by the diffusion of substrate within the biofilm and the internal mass transfer resistance.

### Kinetics of Biofilm

Substrate conversion in a heterogenous bioreactor such as the FBB can be described by the following steps (Fig. 1):

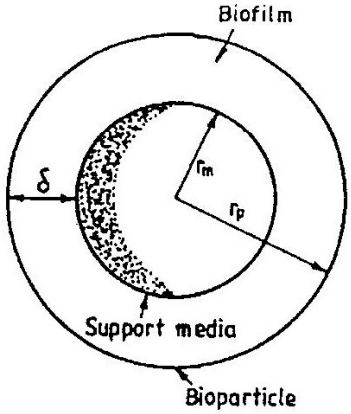


**Fig. 1: Bioparticle schematic.**

1. Transport of substrate from the bulk-liquid to the liquid-biofilm interface (external mass transfer).

2. Transport of substrate within the biofilm (internal mass transfer).

3. Substrate conversion reaction within the biofilm.

Steps 2 and 3 take place simultaneously and thus, neither can be said to control, while step 1 occurs in series with 2 and 3. For intrinsic reaction rates with positive dependence on concentration, the gradients established by steps 1 and 2 decrease the observed reaction rate by decreasing local (i.e. intrabiofilm) substrate concentration. For intrinsic zero order kinetics, steps 1 and 2 can decrease the observed reaction rate by limiting substrate penetration depth into the biofilm.

The significance of an external mass transfer on denitrification rate in the FBB was assessed by Sokol and Halfani [7] using a correlation developed by Mulcahy et al. [8]. It was found that errors in observed rate which resulted if external mass transfer effects were neglected, ranged from 2.6 to 7.1% for bulk-liquid $NO_3^-$-N concentrations over the range 0.04 to 0.006 kg/m$^3$. Errors of this magnitude are acceptable, in light of the greatly simplified mathematics which result. Therefore, the external mass transfer was neglected in the developed model and only the simultaneous intrabiofilm mass transfer and reaction were considered.

The bioparticle continuity equation for limiting substrate is given by formula

$$\frac{D_e}{r^2}\frac{d}{dr}\left(r^2\frac{dS}{dr}\right) = R_{sm} \qquad (1)$$

For intrinsic zero order kinetics, the following reaction rate and boundary conditions apply (Fig. 1):

$$R_{sv} = pk_o \qquad (2)$$

$$S = S_b \quad \text{at } r = r_p \qquad (3)$$

$$(dS/dr) = S = 0 \text{ at } r = r_c \text{ (partial substrate penetration)} \qquad (4)$$

$$(dS/dr) = 0 \text{ at } r = r_m \text{ (full substrate penetration)} \qquad (5)$$

For the partial penetration case, integration of equation (1) yields an expression for substrate penetration depth $r_c$ as follows:

$$\left(\frac{r_c}{r_p}\right)^2 - 1.5\left(\frac{r_c}{r_p}\right)^2 + \left(\frac{1}{2} - \frac{3}{\phi_0^2}\right) = 0 \qquad (6)$$

where:

$$\phi_0 = r_p\left(\frac{\rho k_o}{D_e S_b}\right)^{0.5} \qquad (7)$$

The intrinsic zero order reaction effectiveness factor $\eta_o$ can be defined as the ratio of biofilm volume with substrate concentration greater than zero to total biofilm volume [6]:

$$\eta_o = \frac{1 - (r_c/r_p)^3}{1 - (r_m/r_p)^3} \qquad (8)$$

From equations (6) and (8), it is evident that effectiveness factor $\eta_o$ is a function of $\phi_o$ and the ratio $(r_m/r_p)$. The relationship among these quantities,

using data reported by Mulcahy et al. [6], is shown in Fig. 2.

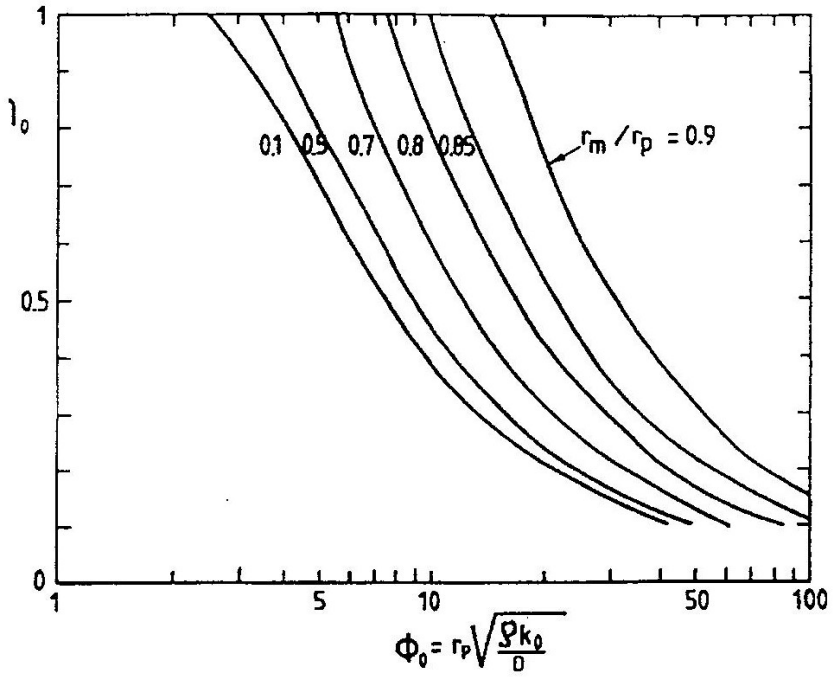


**Fig.2: Bioparticle effectiveness factor $\eta_0$ versus Thiele modulus $\phi_0$ for various ratios of support media radius $r_m$ to bioparticle radius $r_p$ (intrinsic zero order kinetics) for data reported by Mulcahy et al. [6].**

For spherical bioparticles, the dependence on the ratio ($r_m/r_p$) can be eliminated by replacing the particle radius of the conventional Thiele modulus (equation (7)), with a characteristic dimension r defined as:

$$\bar{r} = \frac{Biofilm\ volume}{Biofilm\ exterior\ surface\ area} \qquad (9)$$

or

$$\bar{r} = \frac{\frac{4}{3}\pi\,(r_p^3 - r_m^3)}{4\pi r_p^2} \qquad (10)$$

A modified zero order Thiele modulus can then be defined as follows: Numerical solutions of equations (6), (8) and (11) reported by Mulcahy et

al. [6] are plotted in Fig. 3. It can be seen that for the intrinsic zero order reaction within spherical bioparticles, the use of the modified, in place of the conventional, Thiele modulus results in a linear log-log relationship between $\eta_o$ and $\phi_{om}$. The data are well described by the empirical expression:

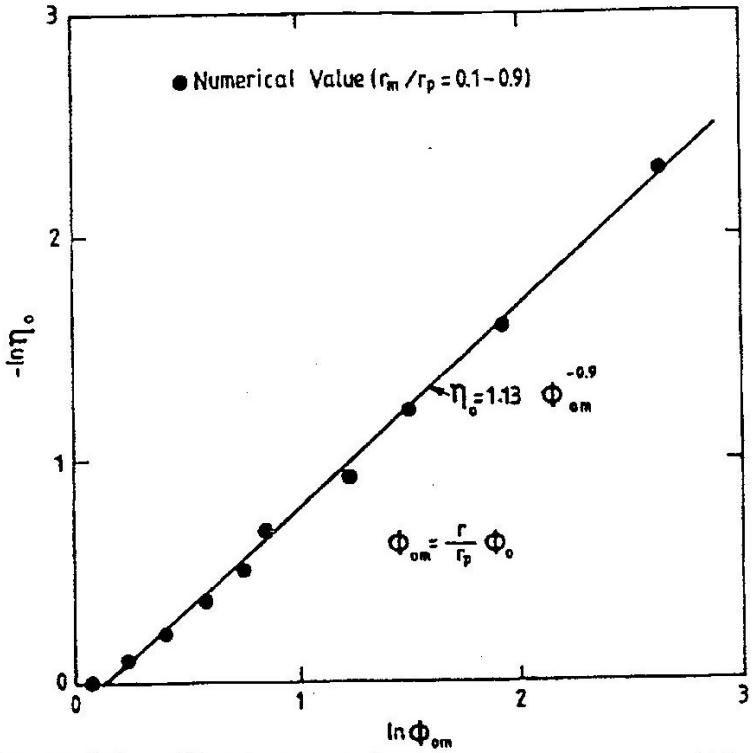


**Fig. 3: Bioparticle effectiveness factor $\eta_o$ versus modified Thiele modulus $\phi_{om}$ (intrinsic zero order kinetics) for data reported by Mulcahy et al. [8].**

$$\eta_o = 1.1302\ \phi_{om}^{-0.9} \tag{12}$$

or substituting the definition of $\phi_{om}$

$$\eta_o = 1.1302 \left[ \bar{r} \left( \frac{\rho k_0}{D_e} \right)^{0.05} \right]^{0.9} S_b^{0.45} \tag{13}$$

Thus, for the intrinsic zero order reaction in partially penetrated bioparticles the effectiveness factor is proportional to the bulk-liquid substrate concentration to the 0.45 power. Setting $\eta_o = 1.0$ in equation 12 gives $\phi_{om}$

= 1.15, the value at which transition occurs from full to partial substrate penetration of the biofilm. For $\phi_{om} < 1.15$ ($\eta_o = 1.0$) the substrate is able to penetrate the entire biofilm thickness and intrinsic zero order kinetics is observed. For $\phi_{om} > 1.15$, the inner portion of the biofilm is substrate-starved and the observed rate is proportional to $S_b^{0.45}$.

Physically, insignificant mass transfer limitations correspond to high bulk-liquid substrate concentration and/or thin biofilm. Conversely, predominant mass transfer limitations are due to low bulk-liquid substrate concentration and/or thick biofilm.

**Model of a FBB**

Liquid phase transport of substrate through the FBB is by combination of convection and axial dispersion. The following simplifications are assumed:

1. No macroscopic radial gradients exist.

2. Bioparticle characteristics are independent of position within the bioreactor.

3. No substrate conversion occurs in the liquid phase (i.e. conversion is limited to bioparticles).

4. Pseudo-steady state conditions exist, i.e. biofilm thickness and biomass concentration are controlled by controlling bed height while maintaining support media volume approximately constant.

For cases in which both convection and axial dispersion are significant, the following equation applies:

$$U\frac{dS_b}{dZ} - D_z\frac{d^2S_b}{dZ^2} + R_{sb} = 0 \qquad (14)$$

with boundary conditions:

$$S_b = S_I \text{ at } Z = 0 \qquad (15)$$

$$\frac{dS_b}{dZ} = 0 \qquad at \qquad Z = H_B \tag{16}$$

For cases in which the dispersion term is negligible, equation 14 simplifies to formula:

$$U\frac{dS_b}{dZ} + R_{sb} = 0 \tag{17}$$

with boundary conditions:

$$S_b = S_I \quad at \qquad Z = 0 \tag{18}$$

Numerical solutions of equation 14 given by Mulcahy et al. [8] for nitrate-N concentrations from 0.003 to 0.03 kg/m$^3$ under typical FBB operating conditions yielded values of the dispersion term that were at all times less than 2% of the magnitude of the corresponding convection term. On this basis, axial dispersion was neglected in the presented model and microscopic convection-reaction was described by the simpler liquid-phase model, i.e. equation 17.

The reaction term $R_{sb}$ of equation 17 describes the observed rate of substrate conversion reaction per unit fluidized bed volume. Considering the heterogeneous nature of the FBB, value of $R_{sb}$ can be more usefully expressed as the product of observed rate per unit biofilm mass $R_{sm}$ and the biofilm mass per unit fluidized bed volume X. Thus, the observed rate $R_{sm}$ is determined as the product of intrinsic rate and effectiveness factor.

For intrinsic zero order kinetics:

$$R_{sm} = \eta_o k_o \tag{19}$$

and

$$R_{sb} = \eta_o k_o X \tag{20}$$

Value of $R_{sb}$ is defined in terms of $S_b$, by substituting the zero order effectiveness factor expression, equation 13 in equation 20 to yields:

$$R_{sb} = 1.1302 k_o X \left( \overline{r} \left( \frac{\rho k_o}{D_e} \right)^{0.5} \right)^{-0.9} S_b^{0.45} \tag{21}$$

**Model Solutions**

For intrinsic zero order systems not limited by mass transfer ($\phi_{om} < 1.15$), effectiveness factor is unity and the overall FBB model is obtained by combining equations 17 and 20. Integration of the resultant expression subject to the boundary condition equation 18, yields the following bulk-liquid substrate concentration profile expression:

$$S_b = S_I - \frac{k_o X Z}{U} \qquad for \qquad \phi_{om} < 1.15 \qquad (22)$$

For intrinsic zero order systems in which mass transfer does limit substrate penetration of the biofilm ($\phi_{om} > 1.15$), the effectiveness factor is given by equation 13 and the overall FBB model is obtained by combining equations 17 and 21. Integration subject to equation (18) yields the following expression:

$$S_b^{0.55} = S_I^{0.55} - \alpha \beta Z \qquad for \qquad \phi_{om} > 1.15 \qquad (23)$$

where

$$\alpha = \frac{X}{U}\left[\frac{3 r_p^2}{\rho^{0.5}(r_p^3 - r_m^3)}\right]^{0.9} \quad \text{and} \quad \beta = 0.6216\, k_o^{0.55} D_z^{0.45}$$

## SIMPLIFIED MODEL OF A FBB

Consider an FBB operated under the steady-state condition in which each spherical media with a uniform size is covered with a uniform layer of biofilm and the liquid is passing upward through the bioreactor in a plug-flow mode, Fig. 4a. The continuity equations of substrate are as follows, Fig. 4b:

**Biofilm phase:**

$$\frac{D_e}{r^2}\frac{d}{dr}\left(r^2 \frac{dS}{dr}\right) = \rho k_o \qquad (24)$$

Boundary conditions:

$$S = S_b \quad \text{at} \quad r = r_p \qquad (25)$$

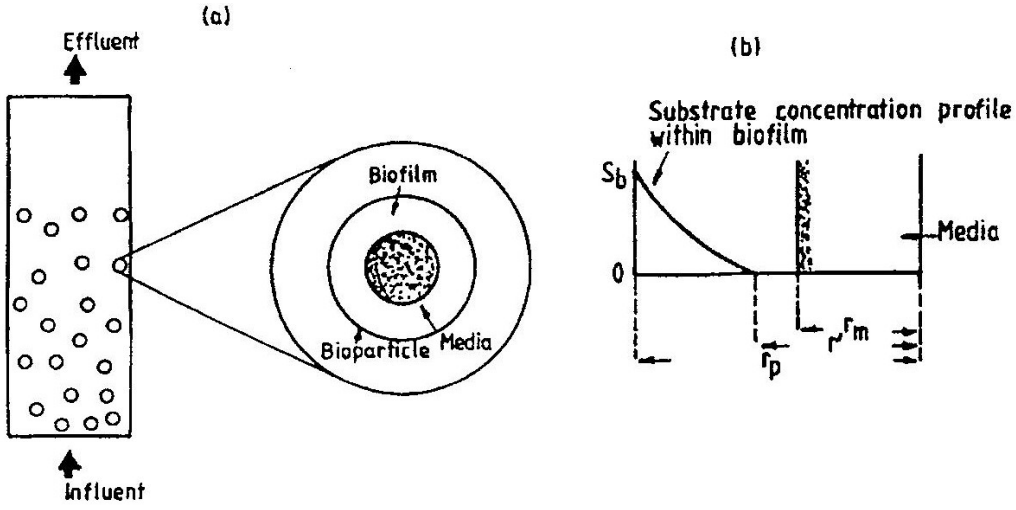


**Fig. 4: (a) Schematic of an FBB and bioparticle; (b) partial penetration of substrate into the biofilm.**

$$\frac{dS}{dr} = 0 \qquad at \qquad r = r' \tag{26}$$

$$S = 0 \qquad at \qquad r = r' \tag{27}$$

**Liquid phase:**

$$U\frac{dS_b}{dZ} + R_{sb} = 0 \tag{28}$$

Boundary condition:

$$S_b = S_I \qquad \text{at} \qquad Z = 0 \tag{29}$$

Integration of equation (24) with boundary conditions (25), (26) and (27) results in equation:

$$1 - \left(\frac{r'}{r_p}\right)^3 = 3.012 \left(\frac{\rho k}{D_e}\right)^{-0.45} (r_p)^{-0.9} S_b^{0.45} \tag{30}$$

or in terms of effectiveness factor $\eta_o$:

$$\eta_o = \frac{1 - \left(\frac{r'}{r_p}\right)^3}{1 - \left(\frac{r_m}{r_p}\right)^3} = \frac{3.012\left(\frac{\rho k}{D_e}\right)^{-0.45} (r_p)^{-0.9}}{1 - \left(\frac{r_m}{r_p}\right)^3} S_b^{0.45} \quad (31)$$

The reaction term $R_{sb}$ in equation 28 is related to the reaction rate occurring within the biofilm by formula:

$$R_{sb} = \eta_o \rho k (1 - \varepsilon) \left[1 - \left(\frac{r_m}{r_p}\right)^3\right] \quad (32)$$

Integration of equation 28, along with equations 29, 30 and 32, yields:

$$S_b^{0.55} = - K\tau + S_I^{0.55} \quad (33)$$

where:

$$K = \frac{1.657 (1 - \varepsilon) (\rho k)^{0.55} D_e^{0.45}}{r_p^{0.9}}$$

and

$$\tau = \frac{Z}{U}$$

Thus, as can be seen from equation 33, the concentration profile of the substrate through the bioreactor can be described by a 0.55 order equation. However, it is important to note that K, a pseudohomogeneous rate coefficient, is actually a parameter rather than a true rate constant. Its value will vary depending on the characteristics of both substrate and biofilm. Among those variable contained in K, only the density and the size of media can be controlled directly by the design engineer. The biofilm thickness and the porosity, under a given set of operating conditions, are dependent on superficial upflow liquid velocity, expanded bed height required or allowed, and media volume. The biofilm dry density, the intrinsic rate constant and the effective diffusivity are not process parameters and can be determined as shown by Shieh [9]. It is worthwhile mentioning that the intrinsic rate constant can be determined only if the mass transfer resistances are eliminated.

The predictions of the model developed in this work were compared with

the operating data of biological denitrification collected from several pilot facilities treating different types of wastewaters. Biomass support media were activated carbon, white silica sand, glass beads and coal. A diameter of the media varied from 0.25 to 0.85 mm and a density from 1,500 to 2,650 kg/m3. It has been concluded by Shieh [9] that, considering a wide range of operating parameters applied in the plants, the data collected were representative also for other denitrification facilities.

Figure 5 shows the substrate concentration profiles as function of residence time for different media size. As can be seen from the figure, there exists an optimal media size that maximizes the substrate conversion rate. Excessive bed expansion associated with the use of small media causes a decrease in the biomass concentration and thus a decrease in the efficiency of the bioreactor. On the other hand, the biomass concentration decreases with increasing media size when a certain media size is exceeded. This results in a decreasing substrate conversion rate.

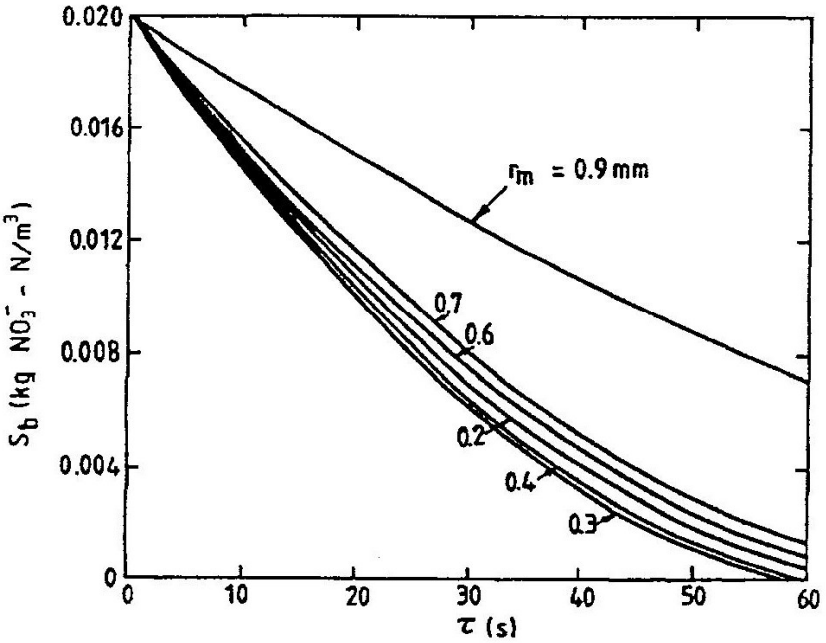


**Fig. 5: Effect of media size (in terms of media radius $r_m$) on the performance of an FBB for data reported by Shieh [9].**

The effect of biofilm thickness on the performance of the FBB is shown in Fig. 6. It can be seen in Fig. 6 that there exists a biofilm thickness that results in a maximum substrate conversion rate. It is interesting to note that neither maintenance of thin biofilm with effectiveness factor of 1.0

(10 to 20 μm biofilm) nor higher biomass concentration (300 μm biofilm) in the bioreactor will be beneficial.

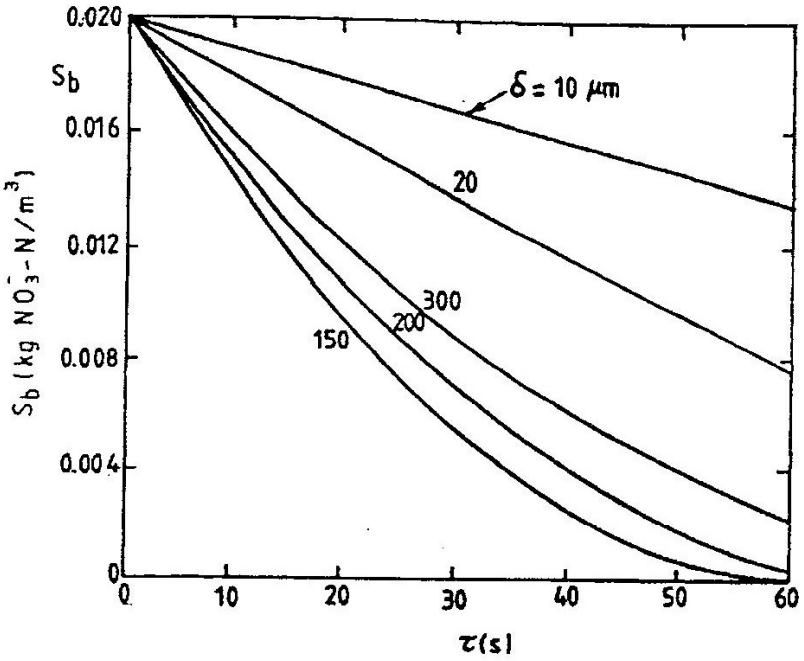


**Fig. 6: Effect of biofilm thickness δ on the performance of an FBB for data reported by Shieh [9].**

The numerical examples reported by Shieh [9] revealed that biofilm thickness and media size are the two most important parameters affecting the performance of FBB. The proposed kinetic model predicts that there exists certain optimal values for these two paraments that maximizes the efficiency of the bioreactor. It is also predicted that the use of denser media in an FBB offers advantages.

The predictions of the simplified model were compared with the operating data of biological denitrification collected from several facilities treating different types of wastewater [7,9]. As stated previously, the substrate profile in an FBB can be described by a 0.55-order equation. Therefore, a linear relationship should be observed if $S_b^{0.55}$ is plotted against τ, providing the model is appropriate for the case studied. Some typical results given by Shieh [9] are shown in Figs 7 and 8. The comparisons presented in the figures show that the simplified model is capable of predicting the results observed in practice. Thus, the model can be applied for design and operation of a fluidised bed bioreactor for removal of carbonaceous matter.

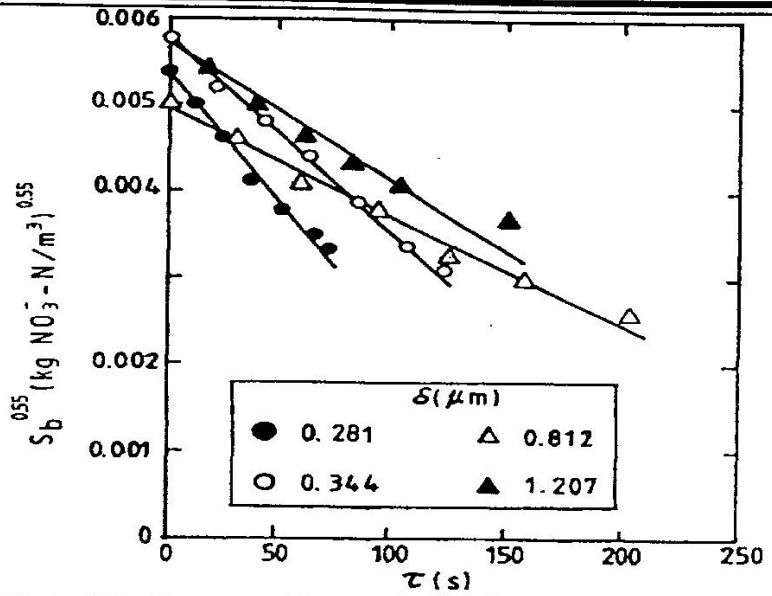


**Fig. 7: Plot of $S_b^{0.55}$ vs. residence time τ for various biofilm thickness δ for data reported by Shieh [9].**

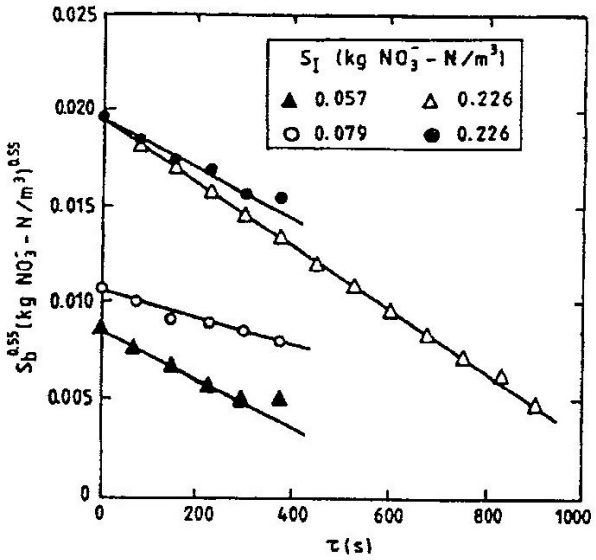


**Fig. 8: Plot of $S_b^{0.55}$ versus residence time τ for various inlet concentrations $S_I$ for data reported by Shieh [9].**

## CONCLUSIONS

From analysis of the presented kinetic models of a fluidised bed bioreactor the following can be concluded:

1. The kinetic model of the biofilm showed that for zero order kinetics, a situation where transition occurs from full to partial substrate

penetration of the biofilm is determined by the value of modified Thiele modulus $\phi_{om}$.

2. When $\phi_{om} < 1.15$, the whole biofilm is active and intrinsic zero order kinetics are observed. For $\phi_{om} > 1.15$, the inner portion of the biofilm is inactive and the observed reaction rate is proportional to the value of $S_b^{0.55}$.

3. The simplified model of the bioreactor was capable of describing the observed bioreactor kinetic behaviour with the accuracy satisfactory for industrial practice. Thus,this model provides a rational basis for design purposes and optimization of a bioreactor.

4. The optimal values of the two most important parameters for efficient performance of the bioreactor, viz. biofilm thickness and media size, that maximize the substrate conversion rate can be determined from the simplied model for a given set of geometric and operating parameters.

## NOTATION

| | |
|---|---|
| $D_e$ | effective diffusion coefficient of substrate in biofilm, $m^2/s$ |
| $D_z$ | axial dispersion coefficient, m/s |
| H | fluidised bed height, m |
| $k_o$ | intrinsic zero order rate constant, kg/(kg s) |
| r | characteristic dimension |
| r | characteristic radius, m |
| $r_c$ | substrate penetration depth, m |
| $r_m$ | support media radius, m |
| $r_p$ | bioparticle radius, m |
| r' | radial distance at which the substrate concentration and its flux cease, m |
| $R_{sb}$ | substrate conversion rate per unit fluidized bed volume, $kg/(m^3\ s)$ |
| $R_{sm}$ | substrate conversion rate per unit biofilm mass, kg/(kg s) |
| $R_{sv}$ | intrinsic substrate conversion rate per unit biofilm volume, $kg/(m^3\ s)$ |
| S | substrate concentration in biofilm phase, $kg/m^3$ |
| $S_b$ | substrate concentration in bulk liquid phase, $kg/m^3$ |
| $S_I$ | inlet substrate concentration, $kg/m^3$ |

| | |
|---|---|
| U | superficial upflow liquid velocity, m/s |
| Z | axial position, m |

*Greek letters*

| | |
|---|---|
| $\varepsilon$ | bed porosity |
| $\delta$ | biofilm thickness, m |
| $\rho$ | biofilm dry density, kg/m$^3$ |
| $\tau$ | residence time, s |
| $\eta_o$ | bioparticle zero order effectiveness factor |
| $\phi_o$ | conventional zero order Thiele modulus |
| $\phi_{om}$ | modified zero order Thiele modulus |

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