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ASSESSMENT OF FINITE DIMENSIONAL APPROXIMATIONS IN INTEGRATION OF SPHERICAL BIOFILMS FOR MICROBIOLOGICAL PROCESSES

In various biotechnological processes such as biodegradation of toxic organic compounds, microorganisms are immobilized on inert carriers. Three-phase fluidized-bed bioreactors and airlift apparata are examples of devices in which microorganisms are immobilized as a thin layer of biomass on fine pellets. Due to a spherical shape of the carrier, the resultant layer of microorganisms has also spherical geometry. In the paper, a quantitative assessment has been made of numerical methods for determining the distributions of reagent concentrations and the effectiveness factors of a biofilm in the form of spherical layers. Calculations have been done for aerobic biodegradation of phenol.

1. INTRODUCTION

Research into the growing mechanism and the properties of a biofilm, i.e. a layer of microorganisms on solid media, has been conducted for approximately thirty years [1, 2], though the phenomenon itself was discovered earlier [3, 4]. Water and sanitary engineering specialists have largely contributed to the advancement of this research. Literature concerning related problems seems to be abundant. Major applications of biofilm engineering, however, are associated with developments in biotechnology when new types of bioreactors were constructed. Monitored biofilm growth with controllable biocenosis is used in such devices as: biofilters, membrane bioreactors and three-phase fluidized-bed and airlift bioreactors with the biofilm grown on fine inert pellets. The paper deals with three methods for numerical simulation of the microbiological processes occurring in biofilms grown on spherical carriers which are often used in three-phase fluidized-bed bioreactors.

Three-phase fluidized-bed bioreactors have been used for multiple implementations. They are employed, among others, in the processes of microbiological degrada-

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tion [5–8]. The advantages of such bioreactors include, above all, highly developed interphase surface, simple design, and first and foremost the separation of the residence time of liquid from that of biomass in the reactors. This enables the hold-up of biomass in the bioreactor for sufficiently high liquid flow rates.

A quantitative description of a microbiological process in a three-phase bioreactor consists of mass balances for the liquid and solid phases. The solid phase is the biofilm grown on an inert carrier. Of particular importance are the balances of the microbiological process in the biofilm, as the latter constitutes an environment in which biochemical processes can take place. The balances are derived in the form of differential equations which describe the distributions of concentrations of species within the biofilm. The effectiveness factor of the biofilm and the average rates of the process within it are determined in this way.

The existing literature, even so famous work as IWA report on biofilm modelling [3], provides no data to assess and compare the efficiency of any quick and relatively simple methods for the integration of biofilms and the calculation of their effectiveness factors. Therefore the so-called finite dimensional approximation which can be used for the calculation of the microbiological processes occurring in biofilms, are discussed and assessed. The methods of orthogonal collocation and finite differences are examined and compared with the shooting method, which is accepted as a reference. The interested reader could easily modify any part of the algorithms in question, and create their own numerical procedures.

The calculations were performed for the aerobic biodegradation of phenol using *Pseudomonas putida* bacteria. The experimentally determined kinetic equations by Seker et al. have been used to describe the uptake rate of the carbonaceous substrate and oxygen [9].

2. MICROBIOLOGICAL PROCESS IN A SPHERICAL BIOFILM AND ITS MATHEMATICAL MODEL

It was shown [10] that an aerobic microbiological process occurring in the biofilm grown on an inert spherical pellet can be described using a system of two non-linear differential equations:

$$\frac{d^2\beta}{dz^2} + \frac{2\delta}{r_0 + \delta z}\frac{d\beta}{dz} - \Phi_{\mathrm{A}}^2 \frac{r_{\mathrm{A}}(\beta,\gamma)}{r_{\mathrm{A}s}} = 0 \tag{1a}$$

$$\frac{d^2\gamma}{dz^2} + \frac{2\delta}{r_0 + \delta z}\frac{d\gamma}{dz} - \Phi_{\mathrm{T}}^2 \frac{r_{\mathrm{T}}(\beta,\gamma)}{r_{\mathrm{T}s}} = 0 \tag{1b}$$

with the boundary conditions:

$$\frac{d\beta(0)}{dz} = \frac{d\gamma(0)}{dz} = 0 \tag{2a}$$

$$\beta(1) = \gamma(1) = 1 \tag{2b}$$

where

$$\beta = \frac{c_{\mathrm{A}}^{b}}{c_{\mathrm{A}s}}, \qquad \gamma = \frac{c_{\mathrm{T}}^{b}}{c_{\mathrm{T}s}}, \qquad \Phi_{\mathrm{A}}^{2} = \frac{\delta^{2} r_{\mathrm{A}s}}{D_{\mathrm{A}e} c_{\mathrm{A}s}}, \qquad \Phi_{\mathrm{T}}^{2} = \frac{\delta^{2} r_{\mathrm{T}s}}{D_{\mathrm{T}e} c_{\mathrm{T}s}}$$

whereas the dimensionless coordinate in the biofilm has been defined as

$$z = \frac{x - r_{\mathrm{o}}}{\delta} \in [0, 1]$$

with x serving as the current coordinate. Reference rates $r_{\mathrm{A}s}$ and $r_{\mathrm{T}s}$ are calculated for concentrations at the biofilm surface.

Uptake rates of carbonaceous substrate and oxygen are determined according to Seker et al. [9] as follows:

$$r_{\mathrm{A}}(\beta, \gamma) = \frac{1}{w_{\mathrm{BA}}} f_1\left(c_{\mathrm{A}}(\beta)\right) f_2\left(c_{\mathrm{T}}(\gamma)\right) \rho_b$$

$$r_{\mathrm{T}}(\beta, \gamma) = \frac{1}{w_{\mathrm{BT}}} f_1\left(c_{\mathrm{A}}(\beta)\right) f_2\left(c_{\mathrm{T}}(\gamma)\right) \rho_b$$

where

$$f_1\left(c_{\mathrm{A}}\right) = \frac{k c_{\mathrm{A}}}{K_s + c_{\mathrm{A}} + \dfrac{c_{\mathrm{A}}^{2}}{K_{in}}}, \qquad f_2\left(c_{\mathrm{T}}\right) = \frac{c_{\mathrm{T}}}{K_{\mathrm{T}} + c_{\mathrm{T}}}$$

The method of orthogonal collocation can be characterized more easily by using the example of a single differential equation. Let us assume then that the following boundary value problem (BVP) should be solved:

$$\frac{d^2 y}{dz^2} + \frac{2\delta}{r_0 + \delta z} \frac{dy}{dz} - \Phi^2 \frac{r_{\mathrm{A}}(y)}{r_{\mathrm{A}s}} = 0 \tag{3}$$

$$\frac{dy(0)}{dz} = 0 \tag{4a}$$

$$y(1) = 1, \qquad z \in [0, 1] \tag{4b}$$

The use of finite dimensional approximation in the form of orthogonal collocation to solve the boundary value problem consists in approximating a function $y(z)$ being the solution of BVP by a polynomial of a certain degree [11]. It is assumed that the polynomials have the following form:

$$y = \sum_{i=1}^{N+1} a_i z^{2i-2} = f(z^2) \tag{5}$$

Polynomials $f(z^2)$ are constructed subject to an orthogonality constraint, i.e. any two of polynomials $f_{m-1}(z^2)$ and $f_m(z^2)$ are required to fulfill the condition:

$$\int_0^1 f_{m-1}(z^2)\, f_m(z^2) dz = 0 \tag{6}$$

Given that $f_0(z^2) = a_0 = 1$, then Eq. (6) provides the basis for determining further polynomials. By doing so, fprmulas have been derived for the first four polynomials which are used throughout this paper:

$$f_1(z^2) = 1 - 3z^2 \tag{7a}$$

$$f_2(z^2) = 1 - 10z^2 + \frac{35}{3} z^4 \tag{7b}$$

$$f_3(z^2) = 1 - 21z^2 + 63z^4 - \frac{231}{5} z^6 \tag{7c}$$

$$f_4(z^2) = 1 - 36z^2 + 198z^4 - \frac{1716}{5} z^6 + \frac{184\,041}{1001} z^8 \tag{7d}$$

Table 1 shows the positive roots of these polynomials. These roots are referred to as internal collocation points. A solution to equation (3) is sought at these points.

Table 1

Positive roots of the polynomials (7)
(internal collocation points)

Polynomial	Collocation points	
$f_1(z^2)$	0.5773502692	
$f_2(z^2)$	0.3399810436	0.8611363116
$f_3(z^2)$	0.2386191861	0.6612093865
	0.9324695142	
$f_4(z^2)$	0.1834346425	0.5255324099
	0.7966664774	0.9602898565

Let $j = 1, 2, ..., N$ be a set of internal collocation points, i.e. the points lying within the interval $z \in [0, 1]$. Then the value of function (5) at the jth collocation point is equal to $y_j = y(z_j)$. The solutions for all collocation points can then be written using vector notation as follows:

$$\mathbf{y} = \mathbf{Q} \cdot \mathbf{a} \tag{8}$$

where the elements of matrix **Q** are calculated as $q_{ji} = z_j^{2i-2}$.

The derivative dy/dz at the collocation point z_j is calculated from the dependence:

$$\frac{dy_j}{dz} = \sum_{i=1}^{N+1} \frac{d}{dz}\left(a_i\, z_j^{2i-2}\right) \tag{9}$$

A single relation can be employed as above to express the derivatives for all collocation points using vector notation:

$$\frac{d\boldsymbol{y}}{dz} = \mathbf{C} \cdot \mathbf{a} \qquad \text{where} \qquad c_{ji} = \frac{d}{dz} z_j^{2i-2} \tag{10}$$

Since $\mathbf{y} = \mathbf{Q} \cdot \mathbf{a}$, then $\mathbf{Q}^{-1} \cdot \mathbf{y} = \mathbf{a}$, thus Eq. (10) can be expressed as follows:

$$\frac{d\boldsymbol{y}}{dz} = \mathbf{C} \cdot \mathbf{Q}^{-1} \cdot \mathbf{y} = \mathbf{B} \cdot \mathbf{y} \tag{11}$$

Second derivative $d^2y/\ dz^2$ at the point z_j, in turn, is defined by the equation:

$$\frac{d^2 y_j}{dz^2} = \sum_{i=1}^{N+1} \frac{d^2}{dz^2}\left(a_i z_j^{2i-2}\right) \tag{12}$$

For all collocation points, we have then:

$$\frac{d^2 \boldsymbol{y}}{dz^2} = \mathbf{D} \cdot \mathbf{a} = \mathbf{D} \cdot \mathbf{Q}^{-1} \cdot \mathbf{y} = \mathbf{G} \cdot \mathbf{y} \tag{13}$$

After substituting the expressions with derivatives of the first and second order into Eq. (3), a system of $N+1$ non-linear algebraic equations is obtained with respect to $y_1, y_2, ..., y_{N+1}$ variables, while $y_{N+1} = y(z_{N+1}) = y(1)$

$$\sum_{i=1}^{N+1} g_{ji} y_i + \frac{2\delta}{r_o + \delta z_j} \sum_{i=1}^{N+1} b_{ji} y_i - \frac{\Phi^2}{r_{As}} r_A(y_j) = 0, \qquad j = 1, 2, ..., N \tag{14a}$$

$$y_{N+1} - 1 = 0 \tag{14b}$$

Coefficients g_{ji} and b_{ji} are the components of predefined matrices **G** and **B**.

The use of the collocation method to determine the concentrations of the carbonaceous substrate and oxygen in the biofilm (Eqs. (1a), (1b)) consists in solving the system of $2(N+1)$ non-linear algebraic equations:

$$\sum_{i=1}^{N+1} g_{ji}\beta_i + \frac{2\delta}{r_o + \delta z_j}\sum_{i=1}^{N+1} b_{ji}\beta_i - \frac{\Phi_A^2}{r_{As}} r_A(\beta_j, \gamma_j) = 0, \qquad j = 1, 2, ..., N \tag{15a}$$

$$\beta_{N+1} - 1 = 0 \tag{15b}$$

$$\sum_{i=1}^{N+1} g_{ji}\gamma_i + \frac{2\delta}{r_o + \delta z_j}\sum_{i=1}^{N+1} b_{ji}\gamma_i - \frac{\Phi_T^2}{r_{Ts}} r_T(\beta_j, \gamma_j) = 0, \qquad j = 1, 2, ..., N \tag{15c}$$

$$\gamma_{N+1} - 1 = 0 \tag{15d}$$

Another finite dimensional approximation is the grid method, or in other words, the method of finite differences. In this approach, a set of points is generated in equal distances h within the integration interval $z \in [0, 1]$. These points make up the nodes of the grid. Equations for the approximation of derivatives are inscribed in the grid nodes and boundary conditions, using appropriate finite differences. If M nodes are placed across an integration interval, the determination of concentration distributions in the biofilm, i.e. the solution of differential problem (1)–(2), is reduced to solving the following system of $2M$ nonlinear algebraic equations:

$$-3\beta_1 + 4\beta_2 - \beta_3 = 0, \qquad i = 1 \tag{16a}$$

$$\frac{\beta_{i+1} - 2\beta_i + \beta_{i-1}}{h^2} + \frac{2\delta}{r_o + \delta z_i}\frac{\beta_{i+1} - \beta_{i-1}}{2h} - \frac{\Phi_A^2}{r_{As}} r_A(\beta_i, \gamma_i) = 0, \quad i = 2, 3, ..., M-1 \tag{16b}$$

$$\beta_M - 1 = 0 \tag{16c}$$

$$-3\gamma_1 + 4\gamma_2 - \gamma_3 = 0, \qquad i = 1 \tag{16d}$$

$$\frac{\gamma_{i+1} - 2\gamma_i + \gamma_{i-1}}{h^2} + \frac{2\delta}{r_o + \delta z_i}\frac{\gamma_{i+1} - \gamma_{i-1}}{2h} - \frac{\Phi_T^2}{r_{Ts}} r_T(\beta_i, \gamma_i) = 0, \quad i = 2, 3, ..., M-1 \tag{16e}$$

$$\gamma_M - 1 = 0$$

where $i = 1, 2, ..., M$ refers to ith grid node.

The efficiency of both finite dimensional approximation methods has been compared with that of the shooting method. Its algorithm has previously been tested for linear kinetics, for which an analytical solution is available. By comparing the analytical results with those obtained using the shooting method it has been confirmed that the latter is sufficiently accurate in the sense that the results with repeatability of even eight significant digits are fully achievable. The tests have demonstrated that the relative error of the shooting method compared to the analytical solution does not exceed $5 \cdot 10^{-5}$%.

To solve the boundary value problem (1)–(2) using the shooting method, let us introduce the following denotations:

$$y_1 = \beta, \qquad y_2 = \frac{dy_1}{dz} = \frac{d\beta}{dz}, \qquad \frac{dy_2}{dz} = \frac{d^2\beta}{dz^2}$$

$$y_3 = \gamma, \qquad y_4 = \frac{dy_3}{dz} = \frac{d\gamma}{dz}, \qquad \frac{dy_4}{dz} = \frac{d^2\gamma}{dz^2}$$

Then the system of Eqs. (1) with conditions (2) can be presented as follows:

$$\frac{dy_1}{dz} = y_2 \tag{17a}$$

$$\frac{dy_2}{dz} = -\frac{2\delta}{r_o + \delta z} y_2 + \Phi_A^2 \frac{r_A(y_1, y_3)}{r_{As}} \tag{17b}$$

$$\frac{dy_3}{dz} = y_4 \tag{17c}$$

$$\frac{dy_4}{dz} = -\frac{2\delta}{r_o + \delta z} y_4 + \Phi_T^2 \frac{r_T(y_1, y_3)}{r_{Ts}} \tag{17d}$$

$$y_2(0) = y_4(0) = 0 \tag{18a}$$

$$y_1(1) = y_3(1) = 1 \tag{18b}$$

To integrate the system of Eqs. (17) within the interval from $z = 0$ to $z = 1$, missing boundary conditions $y_1(0) = x_1$ and $y_3(0) = x_2$ should be assumed, and then it should be verified whether the conditions for $z = 1$ are fulfilled, i.e. whether $y_1(1) = 1$ and $y_3(1) = 1$. Such reasoning reduces the solution of the boundary value problem to solving the system of non-linear equations:

$$f_1(\mathbf{x}) = y_1(1) - 1 \tag{19a}$$

$$f_2(\mathbf{x}) = y_3(1) - 1 \text{ , } \mathbf{x} = (x_1, x_2) \tag{19b}$$

As described here, the shooting method consists of an algorithm to integrate system of differential equations (17) with an imposed superordinated algorithm to solve the system of algebraic solutions (19). The fourth order Runge–Kutta method with the integration step $\Delta z = 0.005$ has been used to integrate Eqs. (17), whereas system of Eqs. (19) has been solved using the Newton method, including numerical calculation of the Jacobi matrix.

3. DISCUSSION OF THE RESULTS

The sought solution to differential equations (1) with boundary conditions (2) are the functions describing the dimensionless concentration of carbonaceous substrate $\beta(z)$ and dimensionless concentration of oxygen $\gamma(z)$ over the biofilm. These functions, also called concentration profiles, indicate possible depletion of particular species inside the biofilm. Its thickness can be controlled on this basis, e.g. to protect microorganisms from anoxia.

The efficiency of the orthogonal collocation method with the shooting one, which is accepted as a reference, is compared in Table 2. A minimum number of internal collocation points N have been selected to determine the application limits of the collocation method. For better clarity, only the function $\beta(z)$ describing the dimensionless carbonaceous substrate concentration has been presented.

Table 2

Distribution of dimensional concentration of carbonaceous substrate in biofilm $\beta(z)$ obtained for $\Phi_A = 3$ by the shooting method and by orthogonal collocation and relative error of orthogonal collocation Δ

z	Shooting method	Orthogonal collocation			
		$N = 2$	Δ [%]	$N = 4$	Δ [%]
0.0	0.0902930	0.1007690	11.6	0.0929365	2.93
0.2	0.1130351	0.1192938	5.54	0.1140572	0.90
0.4	0.1834807	0.1836903	0.11	0.1835787	0.052
0.6	0.3225195	0.3198253	–0.83	0.3226893	0.053
0.8	0.5732899	0.5716100	–0.29	0.5733580	0.012
1.0	1.0000000	1.0000000	0.00	1.0000000	0.00

As appears from Table 2, the selection of only two internal collocation points is sufficient to produce qualitative, and even quantitative estimates as the approximation error does not exceed 1% for coordinate $z \geq 0.4$. Extending the number of the collocation points up to four brings already satisfactory results.

A similar quantitative comparison is provided in Table 3, which shows functions $\beta(z)$ obtained using the method of finite differences. As in the previous case, it has been compared with the shooting method. Two values of the grid nodes have been assumed for calculations, namely: $M = 10$ and $M = 20$. In this case however, the effect of doubling the number of nodes is less effective than in the collocation method. If the number of nodes is increased from $M = 10$ to $M = 20$ in the finite difference method, the approximation error decreases by 3.8% on average, whereas changing $N = 2$ to $N = 4$ in the collocation method reduces such error by tenfold.

Table 3

Distribution of dimensional concentration of carbonaceous substrate in biofilm $\beta(z)$ obtained for $\Phi_A = 3$ by the shooting method and by the finite differences algorithm and relative error of the finite differences method Δ

z	Shooting method	Method of finite differences			
		$M = 10$	Δ [%]	$M = 20$	Δ [%]
0.0	0.0902930	0.09225949	2.18	0.0909143	0.69
0.2	0.1130351	0.1146772	1.45	0.1134991	0.41
0.4	0.1834807	0.1850648	0.86	0.1838998	0.23
0.6	0.3225195	0.3239721	0.45	0.3228925	0.12
0.8	0.5732899	0.5742480	0.17	0.5735327	0.04
1.0	1.0000000	1.0000000	0.00	1.0000000	0.00

As results from Tables 2 and 3, the approximation is the least accurate at the support of the biofilm, i.e. for $z = 0$. The nearer the surface of the biofilm, the more accurate the approximation of concentration distribution becomes. Therefore, apart from comparing the profiles themselves, a measure relating to the biofilm as a whole has to be introduced to assess the approximations used. Such a measure is the effectiveness factor of the biofilm which is calculated from:

$$\eta = \frac{r_{\mathrm{A}av}}{r_{\mathrm{A}s}} \tag{20}$$

where

$$r_{\mathrm{A}av} = \frac{3\delta}{(r_{\mathrm{o}} + \delta)^3 - r_{\mathrm{o}}^3} \int_0^1 (r_{\mathrm{o}} + \delta z)^2 \, r_{\mathrm{A}} \left[\beta(z), \gamma(z)\right] dz \tag{21}$$

As can be seen from the form of Eq. (21) representing the average rate of the bioprocess, it contains information on the entire concentration profiles of both reagents, and therefore it can be used as a reliable measure of accuracy when determining functions $\beta(z)$ and $\gamma(z)$. The effectiveness factors of the biofilm calculated using the shooting and the orthogonal collocation methods are compared in Table 4. A similar comparison to the method of finite differences is given in Table 5. For better clarity, graphical comparison of the results discussed is presented in Fig. 1, where relative error Δ is computed as

$$\Delta = \frac{\eta_{\text{approx.}} - \eta_{\text{shooting}}}{\eta_{\text{shooting}}} \cdot 100\% \tag{22}$$

where $\eta_{\text{approx.}}$ denotes η obtained by any finite dimensional approximation algorithm whereas η_{shooting} means the η calculated by shooting method.

Two conclusions can be drawn from the data presented in Tables 4 and 5 as well from Fig. 1, both of them cognitive and practical in nature:

- The orthogonal collocation method can be used for processes characterized by even large values of the Thiele modulus.
- Doubling the number of nodes when calculating the effectiveness factor of the biofilm is much more effective in the collocation method than in the finite difference method.

Table 4

Effectiveness factors of a biofilm η obtained by the shooting method and by the orthogonal collocation
(Δ means the relative error of the orthogonal collocation)

Φ_A	Shooting method	Orthogonal collocation			
		$N = 2$	Δ [%]	$N = 4$	Δ [%]
0.1	0.99895	0.99897	0.002	0.99896	0.001
0.2	0.99580	0.99588	0.008	0.99583	0.003
0.5	0.97397	0.97445	0.049	0.97414	0.017
1.0	0.89990	0.90162	0.19	0.90048	0.064
2.0	0.68538	0.68874	0.49	0.68602	0.093
3.0	0.51409	0.51476	0.13	0.51451	0.082
5.0	0.33319	0.30869	–7.3	0.33324	0.015
7.0	0.24539	0.18003	–26.6	0.24542	0.012
10.0	0.17565	0.06095	–65.3	0.17572	0.039

Table 5

Effectiveness factors of a biofilm η obtained by the shooting method and by the finite differences algorithm
(Δ means the relative error of the finite differences method)

Φ_A	Shooting method	Method of finite differences			
		$M = 10$	Δ [%]	$M = 20$	Δ [%]
0.1	0.99895	0.99897	0.002	0.99896	0.001
0.2	0.99580	0.99582	0.002	0.99581	0.001
0.5	0.97397	0.97408	0.011	0.97400	0.003
1.0	0.89990	0.90031	0.045	0.90001	0.012
2.0	0.68538	0.68636	0.14	0.68565	0.039
3.0	0.51409	0.51546	0.27	0.51446	0.072
5.0	0.33319	0.33571	0.76	0.33384	0.15
7.0	0.24539	0.24910	1.5	0.24636	0.39
10.0	0.17565	0.18096	3.0	0.17709	0.82

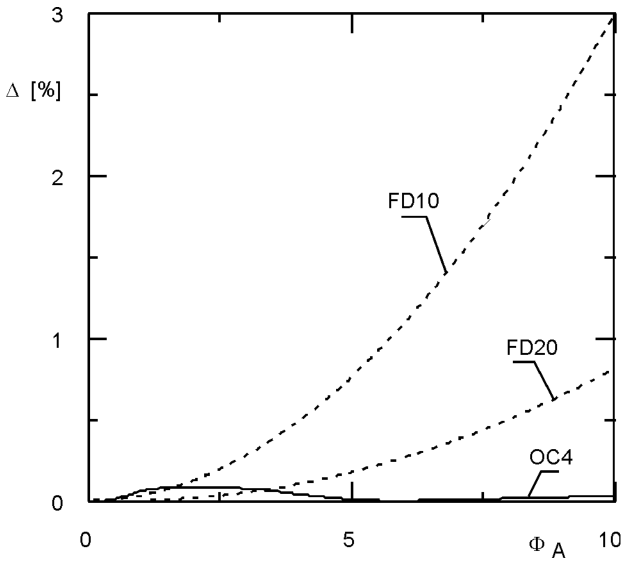

Fig. 1. Relative errors Δ in computing of the effectiveness factor of a biofilm by the orthogonal collocation with four collocation points (OC4) and by the finite difference algorithm with 10 (FD10) and 20 nodes (FD20)

4. CONCLUSIONS

Two finite dimensional approximation methods for integration of models describing biofilms with spherical geometry have been presented. They can be used for the modelling, design, and operational simulations of bioreactors with an immobilized biofilms of microorganisms, both on mobile carriers, such as in fluidized bed or airlift bioreactors, and on fixed carriers that are found in three-phase aerobic bioreactors with packed beds.

Table 6

Relative time of computation required for approximate methods in comparison with the shooting method

Shooting method	Method of orthogonal collocation		Method of finite differences	
$\Delta z = 0.005$	$N = 2$	$N = 4$	$M = 10$	$M = 20$
1	0.122	0.496	0.288	1.255

The efficiency of the approaches under investigation has been assessed quantitatively, both in terms of the accuracy of calculations and the time required for such calculations. Table 6 contains a specification of the relative computation times required in the finite dimensional approximations as compared to the shooting method.

These are the means obtained from the calculations for various values of the Thiele modulus. For instance, the collocation method with $N = 4$ internal points requires 0.496 of the time that is needed for the shooting method. The data in Table 6 also indicates that the method of finite differences with the number of nodes $M = 20$ is 1.255 times slower than the shooting method.

It has been demonstrated that the orthogonal collocation method is advisable for not very large values of the Thiele modulus. Then a sufficiently accurate solution can be obtained within the shortest time. A larger number of collocation points should be used, however, when the values of the Thiele modulus are higher.

All the numerical methods discussed can also be used for the integration of any other objects with spherical symmetry, e.g. fully active biocatalyst pellets. It is then sufficient to assume $r_0 = 0$ in the equations presented above.

SYMBOLS

c_A, c_T	– concentration of carbonaceous substrate A and oxygen T, respectively, kg·m^{-3}
D_e	– effective diffusion coefficient of the biofilm, m^2·h^{-1}
h	– distance between grid nodes
M	– number of nodes in the finite difference method
N	– number of internal collocation points
r_A, r_T	– consumption rate of carbonaceous substrate A and oxygen T, kg·m^{-3}·h^{-1}
r_0	– radius of the inert carrier, m
w_{BA}, w_{BT}	– yield coefficients
z	– dimensionless coordinate in the biofilm
β	– dimensionless concentration of carbonaceous substrate
γ	– dimensionless concentration of oxygen
δ	– biofilm thickness, m
η	– effectiveness factor of the biofilm
ρ_b	– biofilm density, kg B·m^{-3}
Δ	– relative error of finite dimensional approximation tested, %
Φ	– Thiele modulus

SUBSCRIPTS AND SUPERSCRIPTS

A	– limiting carbonaceous substrate
B	– biomass
T	– oxygen
s	– external surface of the biofilm
b	– biofilm

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