Cellular automata-based modelling and simulation of biofilm structure on multi-core computers

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ABSTRACT

The article presents a mathematical model of biofilm growth for aerobic biodegradation of a toxic carbonaceous substrate. Modelling of biofilm growth has fundamental significance in numerous processes of biotechnology and mathematical modelling of bioreactors. The process following double-substrate kinetics with substrate inhibition proceeding in a biofilm has not been modelled so far by means of cellular automata. Each process in the model proposed, i.e. diffusion of substrates, uptake of substrates, growth and decay of microorganisms and biofilm detachment, is simulated in a discrete manner. It was shown that for flat biofilm of constant thickness, the results of the presented model agree with those of a continuous model. The primary outcome of the study was to propose a mathematical model of biofilm growth; however a considerable amount of focus was also placed on the development of efficient algorithms for its solution. Two parallel algorithms were created, differing in the way computations are distributed. Computer programs were created using OpenMP Application Programming Interface for C++ programming language. Simulations of biofilm growth were performed on three high-performance computers. Speed-up coefficients of computer programs were compared. Both algorithms enabled a significant reduction of computation time. It is important, inter alia, in modelling and simulation of bioreactor dynamics.

Key words | biofilm structure, cellular automata, mathematical modelling, parallel algorithms

NOMENCLATURE

Bi Biot number
$c_A, c_B$ mass concentration of the carbonaceous substrate, bacteria and oxygen [kg/m³]
$c_T$ mass concentration of the carbonaceous substrate in stream feeding a bioreactor [kg/m³]
$D_e$ effective diffusion coefficient in biofilm [m²/h]
$f_{par}$ fraction of code that can be parallelized
$j$ number of grids for each substrate
$k$ maximum specific growth rate [1/h]
$k_s$ mass transfer coefficient
$K$ saturation constant [kg/m³]
$K_{in}$ inhibition constant [kg/m³]
$L_b$ thickness of the biofilm [m]
$N_s$ number of iterations required for obtaining pseudo-steady state of concentration’s profiles of the reagents
$P$ number of cores
$P_o$ probability of microorganism decay
$P_{det}$ probability of biofilm detachment
$P_{di}$ probability of diffusion of $i$-th substrate, ($i = A, T$)
$P_{diw}$ probability of diffusion of $i$-th substrate in water ($i = A, T$)
$r_A$ uptake rate of carbonaceous substrate [kg/m³·h]
$r_T$ uptake rate of oxygen [kg/m³·h]
$S$ speed-up coefficient
$t$ time [s], [h]
$T_i$ execution time using $i$ number of cores
$x$ current coordinate in the biofilm [m]
$z$ dimensionless coordinate in the biofilm

Greek symbols

$\Phi$ Thiele modulus for the biofilm
$\delta$ dimensionless concentration of oxygen in the biofilm
$\eta$ dimensionless concentration of carbonaceous substrate in the biofilm

doi: 10.2166/wst.2015.426
Dynamical simulations of complex phenomena occurring in chemical engineering require the use of advanced computer programs. The growing demand for computing power, until recently, was met by increasing the clock frequency of a processor. However, after 2000, the development of this technology has slowed down significantly. For this reason, parallel processing is gaining importance in solving science and engineering problems.

Chemical engineering is a discipline that undoubtedly demonstrates the need for parallel algorithms. This is evidenced by the numerous works listed below concerning the use of parallel programming in this discipline. For example, Linford et al. (2009) carried out a simulation of the chemical reactions system on different parallel architectures. Coon & Stadther (1989) developed a parallel algorithm of LU sparse matrix decomposition. Mukadi & Hayes (2002) used parallel processing for simulating the dynamics of a catalytic reactor. Radeke et al. (2010) used an architecture of graphics processing units (GPUs) for simulating the mixing process of powders.

OpenMP Application Programming Interface (API) is designed for programming a broad range of shared memory architectures. Usage of OpenMP is based on adding special instructions, called directives, to sequential program written in Fortran, C or C++ (Chapman et al. 2008). The major advantages of this API are enumerated below:

- OpenMP is relatively simple to use (Muhammad & Eberl 2010).
- A compiler has the ability to omit OpenMP directives. Then, a source code is compiled into a sequential program (Oliverio et al. 2011).
- Programs can be run on distributed memory architectures, including high-performance computer clusters (supercomputers), working based on the technology of virtual symmetrical processing (vSMP).
- OpenMP reduces the execution time of programs run on personal computers which now often have multi-core processors.

Cellular automata theory is used in simulations of physical, chemical, or biological phenomena, including modelling the structure of biofilms (Hermanowicz 1999; Hunt et al. 2003; Chambless et al. 2006; Chambless & Stewart 2007). Simulations of biofilm dynamics are very time consuming. For example, Muhammad & Eberl (2010) found that a simulation of multi-species biofilm performed using a single computing core can take up to 2,400 minutes. In the same work, the time of parallel computations on different computers with multi-core processors was compared. This comparison shows that the duration of the simulation on different computers is difficult to predict. The conclusion drawn by the authors cited inspired the research described in this paper. The calculations made in this work were carried out on the computing nodes of several high-performance computers. The relationships between speed-up coefficients and the number of computing cores were determined.

The work of Pizarro et al. (2005), concerning biofilm growth by the means of cellular automata, presented an efficient method for increasing computer program performance using a single-core processor. However, the cited work concerned a microbiological process following single-substrate Monod kinetics. The authors proposed a probabilistic manner for modelling substrate utilization. It is not possible to apply such an approach for Haldane kinetics, and moreover, for double-substrate kinetics. Therefore, this work presents an own mathematical model suitable for such kinetic models.

It is commonly believed that cellular automata algorithms offer the possibility for simple parallelization. However, this is true only for so-called synchronous cellular automata. The presented algorithm belongs to the group of asynchronous algorithms. In the literature, there are several
MATERIALS AND METHODS

Description of cellular automata based model

In biofilm models based on cellular automata theory, two different approaches to modelling of diffusion and reaction may be used. In the first, differential equations are used to describe those processes. The work of Picioreanu et al. (1998) and Xavier et al. (2005) are examples. In the second example, the diffusion process is simulated using an algorithm of random walks. This method was used in the work of Pizarro et al. (2001, 2004) and Chang et al. (2003). In the model presented, the second mentioned approach was used. When this approach is used, the dynamics of diffusion and reaction processes are simulated. Hence, such algorithms require considerable computational resources (Chang et al. 2003).

In this paper, two-dimensional overlapping grids were used, as in the work of Pizarro et al. (2001) concerning single-substrate kinetics. Grids for substrates contain information on concentrations of oxygen or carbonaceous substrate, while grids for biomass contain information about the presence and state of microorganisms. In this study, variants with different numbers of grids for substrates were used: one grid for each substrate, two, four and eight. It will be further shown that the number of grids for substrates influences the accuracy of the algorithm. The first two variants are presented in Figure 1. In the model proposed, the von Neumann neighbourhood was used. Periodic conditions were employed on the sides of the grids. At the fixed distance from the front of the biofilm at each iteration, the state of cells in the grids for substrate is set to $c_i^f$ ($i = A, T$). This is to simulate a liquid phase with a constant concentration of oxygen T and carbonaceous substrate A.

Because reaction and diffusion processes occur at a much faster rate than the growth of biofilm, it is assumed that the distribution of concentrations of the reagents reach pseudo-steady state (Pizarro et al. 2001). In the numerical algorithm, it results in a separation of two time steps, of significantly different values. The time step $\Delta t$, of the order of milliseconds, relates to the reaction and diffusion processes, and the $\Delta t_g$ time step, of the order of hours, refers to the processes of growth and decay of bacteria and the detachment of biofilm (Pizarro et al. 2001; Chambless et al. 2006). Such an approach was used in many studies on modelling of biofilms (Tang & Valocchi 2013).

![Figure 1](https://iwaponline.com/wst/article-pdf/72/11/2071/465335/wst072112071.pdf)

Figure 1 | Graphical representation of grids’ and cells’ states; top – one grid for each substrate; bottom – two grids for each substrate; the darker the colour, the larger the concentration of a substrate or biofilm density; white colour denotes cells which are not neighbours of the central cell; B – grid represents the biomass; A, A1, A2 – grids represent the carbonaceous substrate; T, T1, T2 – grids represent oxygen.
The rules used in the model proposed are discussed below.

**Rule 1 – diffusion of substrates**

In this work, the simulation of the diffusion process was done using the algorithm of random walks in a modified version. In the liquid phase, the probabilities of displacement of oxygen mass quantum in all four directions on the grid are the same and equal \( p_{Dtow} \), and the sum of these probabilities is equal to one. The aforementioned modification is the assumption that the probability of displacement of the mass quantum of oxygen is dependent on the presence of biomass in the output and the target cell. It is calculated as follows:

\[
p_{Dt} = p_{Dtow} \cdot \left( \frac{n_w}{2} + \frac{D_{ct} \cdot n_b}{D_{tw} / 2} \right) = 0,25 \cdot \left( \frac{n_w}{2} + \frac{D_{ct} \cdot n_b}{D_{tw} / 2} \right)
\]

(1)

In Equation (1), \( n_b \) is the number characterizing the system of two cells: the start and destination. It specifies the sum of the cells containing the biomass in this pair. It can be one of three values, namely 0, 1 or 2. Whereas \( n_w \) is the number related to the presence of water in the same pair of cells. It also can take values from the set \{0, 1, 2\}.

Similarly, as was done above for the transfer of oxygen, the dependence representing the probability \( p_{da} \) in the simulated domain is as follows:

\[
p_{da} = p_{danw} \cdot \left( \frac{n_w}{2} + \frac{D_{ca} \cdot n_b}{D_{anw} / 2} \right) = 0,25 \cdot \frac{D_{ca} \cdot n_w}{2} + \frac{D_{ca} \cdot n_b}{D_{anw} / 2}
\]

(2)

**Rule 2 – uptake of substrates in biofilm**

The value of the substrate concentration in the cell with indices \((k, l)\) is determined as the arithmetic mean of concentrations in cells with indices \((k, l)\) of each grid for the substrate, according to Equation (3):

\[
c^b_A(k, l) = \frac{1}{f} \sum_{j=1}^{f} c^{bj}_A(k, l)
\]

\[
c^b_T(k, l) = \frac{1}{f} \sum_{j=1}^{f} c^{bj}_T(k, l)
\]

(3a)

(3b)

where \( f \) is the number of grids for each substrate.

Using the equation defining the reaction rate related to the substrate \( A \) and oxygen \( T \), we have:

\[
r^b_A = -\frac{dc^b_A}{dt} \approx \frac{\Delta c^b_A}{\Delta t}
\]

(4a)

\[
r^b_T = -\frac{dc^b_T}{dt} \approx \frac{\Delta c^b_T}{\Delta t}
\]

(4b)

On the basis of the above equation, the expressions for increases in the concentrations of substrates in time step \( \Delta t \) can be determined. These are shown below:

\[
\Delta c^b_A(k, l, t) = -\Delta t \cdot r^b_A\{c^b_A(k, l, t), c^b_T(k, l, t), v_o(k, l, t)\}
\]

(5a)

\[
\Delta c^b_T(k, l, t) = -\Delta t \cdot r^b_T\{c^b_A(k, l, t), c^b_T(k, l, t), v_o(k, l, t)\}
\]

(5b)

The new values of the cell's states for the grids for substrates are:

\[
c^b_A(k, l, t + \Delta t) = c^b_A(k, l, t) + \Delta c^b_A(k, l, t), (j = 1, 2, \ldots, f)
\]

(6a)

\[
c^b_T(k, l, t + \Delta t) = c^b_T(k, l, t) + \Delta c^b_T(k, l, t), (j = 1, 2, \ldots, f)
\]

(6b)

**Rule 3 – Growth and decay of microorganisms and biofilm detachment**

The algorithm of biofilm growth presented in the work of Picioreanu et al. (1998) was implemented. To determine the probability of bacteria decay, the following relationship was used:

\[
p_o = \frac{\Delta t}{\rho_{bio} \cdot \rho_{max}}
\]

(7)

The probability of biofilm detachment was determined using Equation (8) proposed by Chambless & Stewart (2007).

\[
p_{det} = K_{det} \cdot \left| \Delta \rho \right|^2
\]

(8)

In a further part of the work, the comparison of the results obtained using the model based on cellular automata theory with results obtained using the continuous model for
a flat biofilm of fixed thickness was presented. The boundary value problem (9), (10) for a fixed biofilm thickness $L_b = 0.1\, \text{mm}$ was solved using a shooting method. For profiles obtained at stationary conditions, the effectiveness factor of the biofilm was determined. To compare the obtained value of the effectiveness factor, simulations were carried out using cellular automata. They were also performed for the same, fixed thickness of the biofilm. The aforementioned continuous model for the double-substrate process is described by the following equations:

\[
\frac{d^2 \eta}{dz^2} \Phi_A \frac{r^b_A(\eta, \delta)}{r^b_A} = 0 \quad (9a)
\]

\[
\frac{d^2 \delta}{dz^2} \Phi_T \frac{r^b_T(\eta, \delta)}{r^b_T} = 0 \quad (9b)
\]

\[
\frac{d \eta(0)}{d z} = 0 \quad (10a)
\]

\[
\frac{d \delta(0)}{d z} = 0 \quad (10b)
\]

\[
\frac{d \eta(1)}{d z} = \text{Bi}_A (1 - \eta(1)) \quad (10c)
\]

\[
\frac{d \delta(1)}{d z} = \text{Bi}_T (1 - \delta(1)) \quad (10d)
\]

where \( \Phi_A = \frac{L_b^2}{D_{eA} c_A^b} \cdot r_A^b \), \( \Phi_T = \frac{L_b^2}{D_{eT} c_T^b} \cdot r_T^b \), \( \text{Bi}_A = \frac{k_{sA} L_b}{D_{eA}} \), \( \text{Bi}_T = \frac{k_{sT} L_b}{D_{eT}} \).

Dimensionless concentrations in biofilm are defined as:

\[
\eta = \frac{c_A}{c_A^b}, \quad \delta = \frac{c_T}{c_T^b} \quad (11)
\]

Dimensionless coordinate in the biofilm refers to the total thickness of the biofilm, thus:

\[
z = \frac{x}{L_b} \in [0, 1] \quad (12)
\]

Concentrations of both substrates determined by algorithms based on the theory of cellular automata were averaged in rows of grids at any given distance from the base of the biofilm. In this manner, one-dimensional distributions of concentrations were obtained. Subsequently, the biofilm effectiveness factor was calculated by Equation (13) and compared with the value obtained from the solution of the continuous model:

\[
\zeta = \frac{r_{iog}}{r_i}, \quad (i = A, T) \quad (13)
\]

where:

\[
r_{iog} = \int_0^{L_b} r_{iog}^b(x, c_i^b(x)) \, dx, \quad (i = A, T) \quad (14)
\]

Table 1 presents the quantitative comparison of the results of simulations carried out using a different number of grids for substrates $J$ and for different sizes of grid cell. Figure 2 shows the dimensionless profiles of the concentration of substrates obtained using the continuous model (9)–(10) and the discrete model with eight grids for each substrate.

The results presented in Table 1 indicate that with the increasing number of grids $J$ for each substrate, the relative difference between values of the biofilm effectiveness factors calculated according to the two mathematical models decreases. The accuracy of calculations performed according to the mathematical model proposed also increases with the decreasing size of a grid cell.

### Parallel algorithms

The first algorithm is shown in Figure 3 on the example of two grids for each substrate. After the initialization of variables, each core executes the diffusion of substrate...
algorithm for one grid. After the diffusion algorithm, synchronization of threads occurs. Synchronization between threads precludes the appearance of the race condition. Afterwards, the algorithm of utilization of substrates is performed. Both in the algorithm of diffusion and utilization of substrates, the distribution of calculations was performed using the ‘parallel for’ directive. These two algorithms were executed a specified number of times equal to $N_s$, which is equivalent to achieving the pseudo-stationary state of the profiles of reagent concentrations. Then the algorithm related to the growth and decay of microorganisms and biofilm detachment was executed.

The presented algorithm has some disadvantages. The smaller value of the diffusion coefficient of the carbonaceous substrate, and therefore the smaller probability of its diffusion, means that all instructions in the diffusion algorithm are executed less frequently than for oxygen. In the node of synchronization, the less loaded core was expected for the end of calculations performed by the more loaded core. Another disadvantage of this algorithm

![Figure 2](https://iwaponline.com/wst/article-pdf/72/11/2071/465335/wst072112071.pdf)

**Figure 2** Comparison of profiles of reagents obtained using shooting method and cellular automata; in computations eight grids for each substrate were used, cell size was 2 $\mu$m (SM – shooting method; CA – cellular automata).

![Figure 3](https://iwaponline.com/wst/article-pdf/72/11/2071/465335/wst072112071.pdf)

**Figure 3** Algorithm using directives `sections` and `parallel for`; example shown concerns two grids for each substrate and four cores.
was that the increase in the number of cores over $2J$ means that only $2J$ cores perform the diffusion algorithm and redundant cores do not perform any calculations. It is very important because the subroutine based on this algorithm is the most time consuming of all.

Therefore, the second parallel algorithm was created. It is presented in Figure 4. It can be seen that all computing cores are involved in the execution of the diffusion algorithm for grid A1, as well as for the other grids for substrates. For the distribution of the calculations, the ‘parallel for’ and ‘atomic’ directives were used. Using the ‘atomic’ directive eliminated the possibility of the phenomenon of data races, because access to the grid cell at the same time was enabled only for one core.

For evaluation of the parallel algorithms proposed, values of the speed-up coefficients $S$ for different numbers of cores were calculated. Parallel speed-up $S$ is defined as a ratio of the execution time of a program on one core to...
execution time on \( P \) cores (Chapman et al. 2008):

\[
S = \frac{T_1}{T_P} \quad (15)
\]

In an ideal situation, execution time on \( P \) cores should be \( T_1/P \). However, each parallel program has strictly sequential fragments. Increasing the number of cores does not reduce the execution time of those fragments. This relationship is described by Amdahl’s law which can be expressed by the following equation (Chapman et al. 2008):

\[
S = \frac{1}{\left(\frac{f_{par}}{P} + \frac{1}{C_0 \cdot f_{par}}\right)} \quad (16)
\]

Equation (14) shows that when 20% of the program cannot be parallelized, i.e., when \( f_{par} = 0.8 \), the computation time on six cores can be reduced maximally three-fold.

**RESULTS AND DISCUSSION**

The calculations were performed on high-performance computers belonging to PI-Grid infrastructure. Table 2 shows the description of the hardware used.

<table>
<thead>
<tr>
<th>Computer name</th>
<th>Processors</th>
<th>Clock frequency of the processor [GHz]</th>
<th>Number of cores in a node</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZEUS</td>
<td>Intel Xeon E5645</td>
<td>2.40</td>
<td>12</td>
</tr>
<tr>
<td>GALERA</td>
<td>Intel Xeon L5640</td>
<td>2.27</td>
<td>12</td>
</tr>
<tr>
<td>REEF</td>
<td>AMD Opteron 6164 HE</td>
<td>1.70</td>
<td>24</td>
</tr>
</tbody>
</table>

Figure 5 presents the computation time and speed-up coefficients of the calculations versus number of cores used, \( S(P) \). First, we analyzed the results of the program which is an implementation of the algorithm shown in Figure 3, denoted in Figure 5 as ‘Sections’. The maximum number of cores used in the calculation is \( P = 2^J \), which results from the previously described method for the distribution of calculations. Figure 5 indicates that on every multi-core computer, good speed-up coefficients of similar values are obtained. This result differs from the result obtained in the work of Muhammad & Eberl (2010) in which the speed-up coefficients obtained using the same number of cores on different machines differ four-fold.

Unlike the ‘Sections’ algorithm, the usability of the ‘Atomic’ algorithm, presented in Figure 4, is not limited by the relationship \( P = 2^J \). The program implementing the ‘Atomic’ algorithm has been run on cluster Reef, because, among the computers used, its nodes have the biggest number of cores. When 16 cores were used, the speed-up coefficient obtained was \( S = 9 \). In view of the possibility of aggregating nodes into a virtual machine with shared memory, it is possible to use a much larger number of cores than those located in one node. It does not require any modifications in the algorithm and the program.

The values of the speed-up coefficients for the algorithm ‘Sections’ and ‘Atomic’ are high and close to each other, in the range of \( P = 2 \) to \( P = 8 \). The speed-up coefficient for the algorithm ‘Atomic’ with a larger number of cores deviates more from the ideal case, i.e. \( S(P) = P \); however, it allows for further acceleration of the calculations.

Results of the calculations performed include, among others, two-dimensional distributions of biofilm density and concentrations of the substrates. Figure 6 shows...
distributions for the process of the aerobic biodegradation of phenol following the double-substrate kinetics of Seker et al. (1997). The growth time of the biofilm was 2 weeks.

Information on the structure of biofilms formed by phenol-utilizing bacteria comes from several studies concerning fluidized-bed bioreactors (Tang & Fan 1987; Beyenal et al. 1997). In the literature, so far, there is no proposal for a discrete algorithm for the biofilm detachment caused by the collision of particles. As is known, this phenomenon has a significant influence on the biofilm structure. Therefore, to evaluate the proposed model, the data from experiments carried out in a bioreactor with biofilm immobilized on the inner walls of the vessel should be used. For modelling shear detachment in such bioreactors, the algorithm proposed by Chambless & Stewart (2007) can be used, as was done in this study.

For evaluation of the proposed model, the results of Peyton’s (1996) study were used. The quoted study was carried out with the use of Pseudomonas aeruginosa bacteria utilizing glucose for growth. This microbiological process follows the double-substrate Tessier kinetics (Beyenal et al. 2003). A comparison was carried out for the chosen parameters, characterizing the biofilm obtained in laboratory experiments with the results of our own numerical simulations. The thickness of the biofilm, the average density and the surface density in a steady-state for two values of the concentration of carbonaceous substrate in the stream feeding the apparatus were compared. The result of this comparison are shown in Figure 6.

![Figure 6](https://iwaponline.com/wst/article-pdf/72/11/2071/465335/wst072112071.pdf)

**Figure 6** | Distributions of biofilm density (top), phenol (middle) and oxygen (bottom) in biofilm after 2 weeks of growth.

Table 3. It arises from the comparison that the proposed mathematical model gives predictions sufficiently consistent with laboratory experiments.

Two-dimensional distributions of biofilm density obtained in a computer simulation are used for modelling bioreactors with an immobilized biofilm. Moreover, they can be used for the determination of distributions of diffusion coefficients in the biofilm $D_a(x)$. This quantity is generally determined experimentally by comparing the results of experiments with the results of numerical simulations for steady states of biofilm bioreactors. It is, therefore, an expensive and time-consuming process in comparison to the proposed numerical method.

In order to obtain the diffusion coefficients in the biofilm, it was necessary to determine the one-dimensional distributions of the biofilm density with respect to the thickness coordinate in the biofilm. The biofilm density at the distance $x$ from the substratum was calculated as the mean value relative to the total length of the substratum $y$, i.e.:

$$
\rho_b(x) = \frac{1}{y} \int_0^y \rho_b(x, y) dy
$$

(17)

After determination of $\rho_b(x)$ in the above way, diffusion coefficients $D_{a}(x)$ were calculated based on the semi-empirical relationships between these values. The equation proposed by Fan et al. (1990) for Pseudomonas putida may serve as an example:

$$
\frac{D_a(x)}{D_{aw}} = 1 - \frac{0.43 \cdot (\rho_b(x))^{0.92}}{11.19 + 0.27 \cdot (\rho_b(x))^{0.97}}
$$

(18)

The use of this method for determination of the distribution of diffusion coefficients significantly reduces the amount of experimental work.

<table>
<thead>
<tr>
<th>Method</th>
<th>Laboratory experiment</th>
<th>Computer simulation</th>
<th>Laboratory experiment</th>
<th>Computer simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quantity</td>
<td>$\rho_b$ [kg/m³]</td>
<td>$\rho_b$ [kg/m³]</td>
<td>$\rho_s$ [g/m²]</td>
<td>$\rho_s$ [g/m²]</td>
</tr>
<tr>
<td>$L_b$ [μm]</td>
<td>31.0</td>
<td>30.0</td>
<td>20.0</td>
<td>20.0</td>
</tr>
<tr>
<td>$\rho_b$ [kg/m³]</td>
<td>51.61</td>
<td>48.78</td>
<td>42.50</td>
<td>42.55</td>
</tr>
<tr>
<td>$\rho_s$ [g/m²]</td>
<td>1.60</td>
<td>1.46</td>
<td>0.85</td>
<td>0.85</td>
</tr>
</tbody>
</table>
CONCLUSIONS

The paper presents a mathematical model of biofilm growth based on the theory of cellular automata. As the process example, the aerobic biodegradation of phenol was chosen. The aerobic process with substrate inhibition has not been, up to now, a subject of any work concerning modeling using cellular automata.

Mathematical modelling of biofilm growth using discrete models allows determination of its spatial heterogeneity; however, it requires relatively high computing resources. Because of this, in theoretical research concerning this phenomenon, the efficiency of computer programs is an important issue. In view of the fact that nowadays personal computers have multiple computing cores, a significant reduction of computation time can be obtained by the use of parallel processing.

Two parallel algorithms have been proposed and discussed, varying in the distribution of calculations. Computer simulations were performed on three clusters belonging to PL-Grid infrastructure. The algorithms created made it possible to significantly increase the speed of calculation. Parallel programs are designed to run on machines with shared memory. This gives the possibility of execution on commonly used multi-core personal computers and virtual machines with shared memory. It was shown that use of the algorithm based on the Sections directive makes it possible to reduce computation time over five-fold compared to the sequential algorithm. Moreover, computation time will decrease nine-fold if calculations are performed with the use of the algorithm based on the Atomic directive. The relationships between the speed-up coefficient and the number of cores are similar, regardless of which multi-core computer was used for a simulation.

The model presented can be used in theoretical studies on the morphology of biofilms in which the process follows double-substrate kinetics with substrate inhibition. To date, such studies have not been conducted. Two-dimensional distributions of the biofilm density obtained in a computer simulation can be used for modeling a bioreactor with immobilized biofilm and for determination of the distribution of diffusion coefficients in the biofilm. The presented method of modelling of biofilm morphology may be an alternative method for determining the basic quantities characterizing biofilms, thereby reducing the amount of work involved in time-consuming laboratory experiments.

The advantage of modelling all the phenomena occurring in the biofilm in a discrete way is the possibility of simulating the growth of biofilm with complex geometry. Such geometry is observed for real biofilms, for example in biofilters. The mathematical model and algorithms can be used for simulation of other reaction-diffusion processes. In addition, the results can be the basis for the design of parallel algorithms for other mathematical models based on the theory of cellular automata.

ACKNOWLEDGEMENT

This research was supported in part by PL-GRID infrastructure.

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First received 11 May 2015; accepted in revised form 30 July 2015. Available online 14 August 2015