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A Modified Approach to an Analytical Solution of a Diffusion Model for a Biotechnological Process

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Abstract: Biotechnological processes are objects with distributed parameters characterized by a complicated structure of organization and interdependent characteristics. Partial differential equations are used for their behavioural description with modelling in relation to diffusion phenomena considered in this paper. Furthermore, an application of the theory of partial differential equations to obtain a direct analytical solution of the model is considered. This is in contrast with less direct approaches in the literature. The behaviour of the model developed here accords well with real phenomena.

Keywords: Continuous Biotechnological Processes, Distributed Parameters Objects, Partial Differential Equations.

INTRODUCTION

Biotechnological processes (BTP) are characterized by complicated reactions and interdependent characteristics which lead to complicated mathematical descriptions. In order to develop a more complete and precise model, space distribution of the process variables can be considered and included in the model. This determines the behavioural description of BTP as objects with distributed parameters (ODP), using partial differential equations (PDE) or systems of PDEs. The processes in general have wide application in biology and medicine, for instance, in determining erythrocyte sedimentation rates (Reuben and Shannon 1990).

The modelling of BTP as ODP has not been widely studied. In most studies the authors have chosen some method, for example finite differences or orthogonal collocation, to represent the PDE with a finite number of ordinary differential equations. Bourrel et al. (1998) have merely considered the processes in steady-state. Babary et al. (1993) and Julien et al. (1995) have applied the orthogonal collocation method. Dochain et al. (1997) and Jacob, Pingaud et al. (1996) have exploited the methods of both finite differences and orthogonal collocation. Jacob, Lann et al. (1996) have also applied the method of lines and the orthogonal collocation method. The PDE have been approximated by a system of ordinary differential equations in all these studies. To overcome the approximation errors in such approaches one possible way is to use the PDE directly. Hence an elaboration of some new methods and approaches for the description and control of biotechnological process is appropriate.

The twofold aim of this paper is both to model substrate space distribution for a specific class of biotechnological processes, and to obtain an analytical solution of the PDE in the model.

STATEMENT OF THE PROBLEM

A class of fixed bed biotechnological processes is considered wherein the active biomass is kept within the vessel, while the substrate and product flow through it (Babary et al. 1990, 1993). This type of bioreactor is called a biofilter (Figure 1). The problem is to describe the process as an object with distributed parameters and thus to obtain a model of a specific class of BTP.

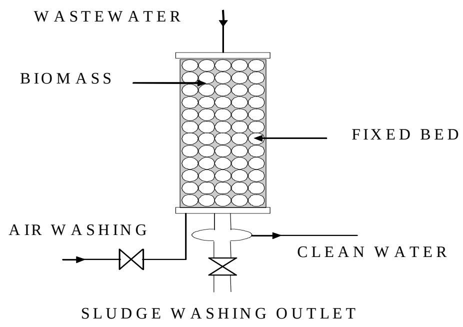

Figure 1: A fixed bed bioreactor

The non-uniformly distributed media elements on the apparatus cross-section, as well as the presence of turbulent diffusion, are expressed as follows (Schmalzriedt et al. 1995):

$$\frac{\partial c}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(ru_r c) + \frac{\partial}{\partial z}(u_z c) = \frac{1}{r}\frac{\partial}{\partial r}\left(D_{eff} r \frac{\partial c}{\partial r}\right) + \frac{\partial}{\partial z}\left(D_{eff}\frac{\partial c}{\partial z}\right) + \\ + reaction + mass\ transfer\ gas/liquid \tag{1}$$

where c is a differentiable function to describe concentration; r, z are radial and axial co-ordinates, respectively; D_{eff} is the turbulent diffusion coefficient, and u_r, u_z are radial and axial components of the rate vector.

In fact Equation 1 represents the equation for the material balance of the concentration. The material balance of the substrate S can be considered in the following two cases:

- when the diffusion of substrate S is regarded as negligible, and
- when the diffusion of S is accounted for in the axial direction.

The first case when diffusion of the substrate S is regarded as negligible has been presented previously (Pencheva et al. 2003; Pencheva 2003). In this paper, the latter, more complicated, case is discussed.

MODELLING OF THE SUBSTRATE

When the space distribution of the substrate S is considered at this stage, the diffusion in one direction, (for example, axial), is given, while the variables do not change in the other direction (Babary et al. 1990, 1993). According to Babary et al. (1990, 1993), the turbulent diffusion coefficient D_{eff} is considered to be a constant and the mass transfer from a gas to a liquid phase is not examined. As was demonstrated in Pencheva et al. (2003) based on (Babary et al. 1990, 1993), the axial component of the rate vector u_z can be expressed as:

$$u_z = \frac{F}{B} \tag{2}$$

where F is the flow rate, constant in the considered direction, via the bioreactor cross-section B. The reaction in the system when the substrate S is modelled is presented as follows (Farlow 1982):

$$\text{reaction} = -k\mu(S)X \tag{3}$$

where X is a differentiable function to describe the biomass concentration [g/l], $\mu(S)$ is a specific growth rate of the biomass, and k is a yield coefficient. This relation describes the biochemical mechanism in the system, expressed as the substrate decrement due to biomass accumulation in the culture medium.

When the biomass X is modelled, the reaction of the system can be presented as follows:

$$\text{reaction} = (\mu(S) - k_d)\, X \tag{4}$$

where k_d is a death coefficient of the biomass, $[h^{-1}]$. The kinetics for the specific growth rate of the biomass are assumed to be:

$$\mu(S) = \mu_{max} \frac{S}{k_S + S} \tag{5}$$

where μ_{max} is the maximum value of $\mu(S)$ $[h^{-1}]$, and k_S is a saturation constant [g/l].

Thus, on the basis of Equations 1–3 and Equation 5, the following parabolic model is obtained for the substrate space distribution, when the diffusion phenomena are considered:

$$\frac{\partial S}{\partial t} = D_{eff} \frac{\partial^2 S}{\partial z^2} - \frac{F}{B}\frac{\partial S}{\partial z} - k\mu_{max} \frac{S}{k_s + S} X \tag{6}$$

The other basic biochemical variable when modelling BTP is the concentration of biomass. Due to the fixed bed reactor, the cell biomass is uniformly distributed in the cultural medium. Therefore, the variation of biomass will be examined in relation to time only:

$$\frac{dX}{dt} = \left[\mu_{max} \frac{S}{k_s + S} - k_d\right] X \qquad 0 \le z \le H \tag{7}$$

Hence, Equations 6 and 7 constitute the mathematical model which describes the BTP in a biofilter as an ODP when the diffusion phenomena are taken into account. When BTP are described as an ODP, the initial conditions should be specified and in this case they can be given as follows:

$$S(z, 0) = S_0 e^{-z^2/b} \quad \text{and} \quad X(0) = X_0 \tag{8}$$

where S_0 and X_0 are the initial concentrations and b is a constant.

The families of curves, which represent the numerical solution of the model in Equations 6–7 by the method of lines are given in Figures 2 and 3 for the substrate and biomass, respectively. The results indicate that the model described by Equations 6 and 7 predicts behaviour similar to a real biotechnological process.

SOLUTION OF THE MODEL

There are two fundamental approaches when BTP are examined as an ODP: in the first one, the PDE, which describe the mathematical model of the processes, are approximated by ordinary differential equations. Most authors have chosen some method, for example, finite differences or orthogonal collocation, to represent the PDE with a finite number of ordinary differential equations (Babary et al. 1990, 1993; Dochain et al. 1997; Jacob, Pingaud et al. 1996; Jacob, Lann et al. 1996; Julien et al. 1995). In this way BTP are presented in a standard form and conventional control theory can be applied. However, the application of this approach leads to the introduction of approximation errors. Other authors (Balakrishnan 1976; Pencheva 2003) have applied the theory of semi-group linear restricted operators, but in this paper the theory of PDE is used directly.

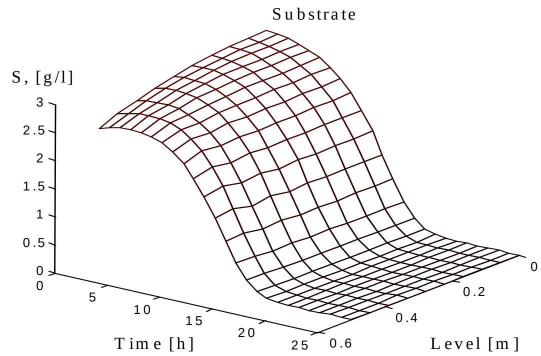

Figure 2: Numerical solution of space distribution of substrate concentration

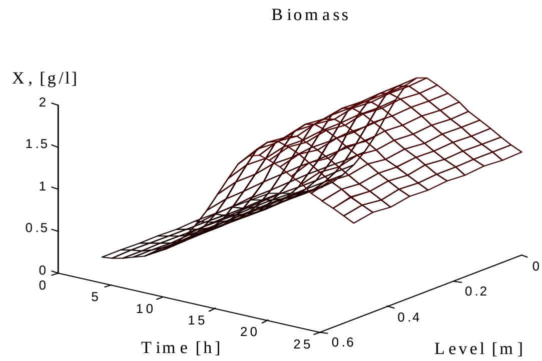

Figure 3: Numerical solution of space distribution of biomass concentration

Equation 6, which describes the concentration of the substrate S, is in fact a non-homogeneous non-linear equation of convective diffusion. So to obtain an analytical solution of this equation a new modified approach, based on existing methods, has to be developed. This approach is based on a transformation of the equation for convective diffusion into the simpler equation for heat conductivity. This modified approach consists of the following steps (Pencheva 2003):

Step 1. According to the theory of PDE, in order to obtain a solution of a given non-homogeneous equation, one first needs the corresponding homogeneous equation to be considered under non-homogeneous initial conditions.

Step 2. For a solution of the corresponding homogeneous equation a modified approach is then used, consisting of the following steps:

Step 2.1. transformation of the initial equation of convective diffusion to the much simpler equation for heat conductivity, using the following relation:

$$S\left(z,t\right) = e^{\frac{u\left(z-\frac{ut}{2}\right)}{2D_{eff}}} f\left(z,t\right) \tag{9}$$

where $f(z,t)$ is a solution of the heat conductivity equation.

Step 2.2. solution of the equation for heat conductivity.

Step 2.3. solution of the initial equation for convective diffusion based on *Step 2.2.*

Step 3. The final step involves obtaining a solution of the initial equation for convective diffusion as a non-homogeneous equation examined under homogeneous initial conditions. Additional difficulties spring from the fact that the non-homogeneity in the equation introduces a non-linearity as well. The general solution of the non-homogeneous equation is the sum of the results from *Step 2* and *Step 3.*

The homogeneous equation, which corresponds to (6), can be given in a general-type formula:

$$S_t = D_{eff} S_{zz} - u S_z \quad \text{where} \quad S_t = \frac{\partial S}{\partial t}, \quad S_z = \frac{\partial S}{\partial z} \quad \text{and} \quad S_{zz} = \frac{\partial^2 S}{\partial z^2} \tag{10}$$

Therefore, by the application of the transformation (9), the solution of (6) is contracted to the solution of the heat conductivity equation. On the basis of the theory of PDE, the following solution of heat conductivity equation is then obtained:

$$f\,(z,t) = \frac{1}{2\sqrt{\pi D_{eff} t}} \int_{-\infty}^{+\infty} \varphi(\xi)\, e^{-\frac{(z-\xi)^2}{4D_{eff}\,t}}\; d\xi \tag{11}$$

where $\varphi(\xi)$ is the initial condition for the heat conductivity equation, which overlaps with the initial condition of the corresponding homogeneous equation (10) which, in turn, corresponds to (6). When the initial condition is as described in (8) and the solution obtained for the heat conductivity equation is replaced in (9), the solution of (10) is:

$$S(z,t) = e^{\frac{-\frac{F}{B}[z-\frac{Ft}{2B}]}{2D_{eff}}} \cdot \frac{S_0}{2\sqrt{\pi D_{eff} t}} \int_0^H e^{-\xi^2 - \frac{(z-\xi)^2}{4D_{eff}\,t}}\; d\xi \tag{12}$$

The relation (12) represents a solution of the homogeneous equation (10), corresponding to the non-homogeneous equation (6), considered under non-homogeneous initial conditions. In terms of the theory of PDE to obtain a solution of the non-homogeneous equation (6), it is necessary to examine the non-homogeneous equation (6) under homogeneous initial conditions. Consequently the general solution is presented as a sum of the two cases and is given as follows:

$$\begin{aligned} S(z,t) = {} & \frac{S_0}{2\sqrt{\pi D_{eff} t}} e^{\frac{-\frac{F}{B}[z-\frac{Ft}{2B}]}{2D_{eff}}} \int_0^H e^{-\xi^2 - \frac{(z-\xi)^2}{4D_{eff}\,t}}\; d\xi \quad + \\ & \int_0^t \int_{-\infty}^{+\infty} \frac{1}{2\pi\sqrt{D_{eff}(t-\tau)}} [-k\mu_{max} \frac{S}{k_s + S}\, X(\tau)]\; e^{-\frac{(\xi-z)^2}{4D_{eff}(t-\tau)}}\; d\xi\; d\tau \end{aligned} \tag{13}$$

If the following assumption, which is meaningful from a biotechnological point of view, is also accepted:

$$\frac{S}{k_S + S} \leq \frac{S_0}{k_S + S_0} = \mu_L \tag{14}$$

then the solution of (13) comes down to the following final form:

$$S(z,t) = \frac{S_0}{2\sqrt{\pi D_{eff} t}} e^{\frac{-\frac{F}{B}[z-\frac{Ft}{2B}]}{2D_{eff}}} \int_0^H e^{-\xi^2 - \frac{(z-\xi)^2}{4D_{eff}\,t}}\; d\xi - \frac{\mu_L k \mu_{max}}{\sqrt{\pi}} \int_0^t X(\tau)\, d\tau \tag{15}$$

The solution of (15), when the values of the biomass numerical solution are given, is shown in Figure 4. Although the values of the constants used for the numerical solution represented in

Figure 2, and those used for the analytical solution (Figure 4), are the same, it can be seen that both figures do not correspond closely. The differences are due to the assumption (14), which allows an analytical solution to be developed, but partly eliminates the non-linearity of the model.

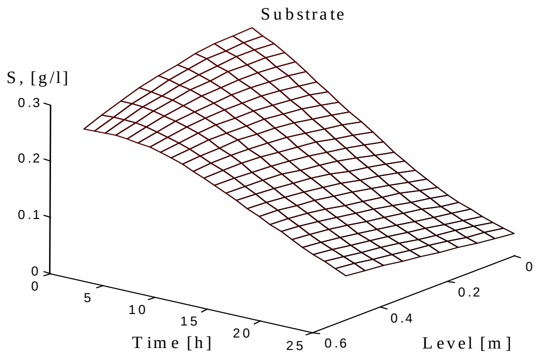

Figure 4: Analytical solution of space distribution of substrate concentration

This type of family of curves, which represents the analytical solution in Equation 15, illustrates that the model obtained behaves similarly to a real biotechnological process. Moreover, it represents the effective application of the modified mathematical approach using the theory of partial differential equations to obtain an analytical solution of the model.

The basic aim of this paper is to present a modified mathematical approach using the theory of partial differential equations for obtaining an analytical solution of the model with the rendering of the substrate diffusion. It is interesting to note that after the comparison and the statistical evaluation (Pencheva 2003), it is found that the differences between the results obtained with and without the rendering of the diffusion phenomena are less than 7% for the substrate and less than 15% for the biomass. At the same time, rendering of the diffusion phenomena leads to a more difficult mathematical description. Therefore, where it is not essential, diffusion phenomena in the system can be regarded as negligible without loss of generality.

CONCLUDING COMMENTS

The following conclusions can be summarised from the foregoing:

§ The equation of material balance of the variable S, which describes the variation of the substrate in the biotechnological processes in a biofilter, with regard to diffusion phenomena, has been derived. The distribution of biomass concentration in the culture medium is uniform because of the fixed bed bioreactor.

§ The numerical solution of the mathematical model of substrate space distribution, presented by the method of lines, demonstrates that the model displays behaviour similar to a real biotechnological process.

§ By applying the developed modified approach within the theory of PDE, the analytical solution of the mathematical model of the substrate space distribution has been found.

§ The analytical solution achieved also shows the efficiency of the direct application of the theory of PDE without resorting to other, less direct, mathematical methods.

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