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Application of the substrate consumption rate to the monitoring of distributed parameter bioreactors

by

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Abstract: This paper deals with the idea of estimation of the substrate consumption rate at each point of the tube of the classical distributed parameter bioreactor and its application to the monitoring of this system. It is shown how to approximate the profile of this parameter on the basis of the orthogonal collocation method and the recursive least-squares procedure with adjustable forgetting factor. Then, it is suggested how to apply this profile for monitoring of the bioreactor work (calculation of the current mass flux of the substrate being reacted in the reactor tube and of the total mass of the substrate reacted in the bioreactor tube during its activity). The idea presented in this paper was validated by means of the computer simulation and the results proving its very good performance complete the paper.

Keywords: biotechnology, distributed parameter systems, least-squares estimation.

1. Introduction

Biotechnological processes have been the subject of growing interest for last several years and publications dealing with this field can be found in relevant journals, e.g. Bogle et al. (1996), Kanai et al. (1996), Shimizu (1996).

Bioreactors have been widely used in wastewater treatment due to the fact that the microorganisms, placed on a fixed bed in a tube, consume harmful nutrients as the water to be treated flows through the reactor. Tubular fixed-bed bioreactors, aimed at cleaning wastewater or improving the quality of drinking water, have emerged as an important treatment method (Pujol et al., 1993).

In majority of suitable publications the outlet substrate concentration is considered as the most important parameter characterizing the quality of the bioreactor work (Dochain et al., 1992; Benthack et al., 1996; Dochain et al., 1997; Czeczot et al., 1999; Babary et al., 1999). In some cases this quantity can be successfully measured and controlled. However, especially in the case of industrial bioreactors working as a part of a wastewater treatment plant, the total mass of the substrate, being reacted due to the biological reaction taking place, is the very important parameter characterizing the biodegradation process. Therefore the idea of monitoring of the biological reaction taking place inside the bioreactor provides the information dealing both with the intensity of the reaction itself and with the possibility of the optimal control of the total mass of the substrate being reacted during bioreactor activity.

The objective of this paper is to describe a methodology for monitoring of the bioreactor in the case of a single substrate. The system is modeled by a set of two PDE's which describe the dynamics of the biomass and of the substrate, respectively. The growth of the biomass is described via the Contois model (Contois, 1959). Then, the resulting nonlinear model is approximated by a set of ordinary differential equations (ODE's) via the orthogonal collocation method (Villadsen and Michelsen, 1978).

In order to enable monitoring of the bioreactor there is a need to define the substrate consumption rate and to propose the procedure for estimation of its value since this parameter cannot be measured directly. In Czeczot (1995) the substrate consumption rate was applied for the first time but the procedure for estimation of its value was based on the substrate concentration measurements with sensors located equidistantly. In this paper the substrate concentration sensors are located at collocation points which ensures the best observability of the process (Damak et al., 1992; Dochain et al., 1997; Waldraff et al., 1998). This approach combines high approximation accuracy with relatively low number of sensors and therefore it is frequently used in practice. Moreover, the procedure for estimation of the substrate consumption rate applies the recursive least-squares method which allows us to minimize the influence of the measurement noise on the estimation accuracy by adjusting the value of the forgetting factor (Czeczot, 1997, 1998; Czeczot et al., 1999).

This paper is organized as follows. The process model is shortly described in Section 2. Then the approach to the idea of the substrate consumption rate is introduced in Section 3. Estimator equations for the substrate consumption rate, derived in discrete-time form, are presented in Section 4. The methodology for monitoring of the bioreactor is described in Section 5. Finally (Section 6) the simulation results show very good performance of the monitoring methodology,

2. Mathematical model of the process

The mathematical model of the system includes dynamic equations for the biomass $X(z,t)$ [g/m^3] and for the substrate $S(z,t)$ [g/m^3] concentrations. A hyperbolic model considered in this paper assumes that the substrate diffusion in the axial direction is negligible, which is acceptable for a class of bioreactors. Consequently, the mass balance equations give the following model (Bastin and Dochain, 1990; Babary et al., 1991):

$$\frac{\partial S(z,t)}{\partial t} = -\frac{w(t)}{L}\frac{\partial S(z,t)}{\partial z} - k_1\mu(z,t)X(z,t) \tag{1}$$

$$\frac{\partial X(z,t)}{\partial t} = [\mu(z,t) - k_d]X(z,t) \tag{2}$$

$$\text{boundary conditions } S(0,t) = S_{\text{in}}(t),\ X(0,t) = X(1,t) = 0 \tag{3a}$$

$$\text{initial conditions } S(z,0) = S_0(z),\ X(z,0) = X_0(z) \tag{3b}$$

with

$z \in [0,1]$ [-] — normalized dimensionless space variable

$w(t)$ [m/h] — velocity of the flowing medium

L [m] — length of the reactor tube

k_1 [-] — yield coefficient

k_d [1/h] — death coefficient.

It is assumed that the microorganisms are concentrated only inside the bioreactor tube and they are placed on a fixed bed. Therefore, equation (2) has the incomplete form without a term describing the convection phenomena. It also results in the assumption that there is no biomass in the inlet and outlet flow so there is no need to apply any boundary conditions to the equation (2) describing the biomass concentration.

The PDE system (1)—(3) is strongly nonlinear due to the nonlinear characteristics of the specific growth rate $\mu(z,t)$ modeled by the Contois expression (Contois, 1959):

$$\mu(z,t) = \mu_{\max}\frac{S(z,t)}{K_c X(z,t) + S(z,t)} \tag{4}$$

with

$\mu_{\max}$ [1/h] — maximum specific growth rate

K_c [-] — saturation coefficient.

Let us note that the mathematical model of the system (1)–(4) describes only the biomass and one substrate concentrations. Although this model is simplified the aim of this work consists in the monitoring methodology. Therefore, this simplified model allows us to concentrate on the methodology that is suggested in the further part of the paper. Moreover, since this methodology is very general it can be easily adapted to the systems, which must be described by much more complicated mathematical models that include for instance the effect of the temperature, pH and/or metabolic concentration.

3. Theoretical approach to the substrate consumption rate

In order to introduce the idea of the substrate consumption rate let us rewrite the equation (1) and present it in the following general form:

$$\frac{\partial S(z,t)}{\partial t} = -\frac{w(t)}{L}\frac{\partial S(z,t)}{\partial z} - r(z,t) \tag{5}$$

with

$$r(z,t) = k_1\mu(z,t)X(z,t)\ [\mathrm{g/m^3\ h}] \text{ — substrate consumption rate.} \tag{6}$$

The value of $r(z,t)$ describes the intensity of the biological reaction taking place at each point of the reactor tube. This approach was applied for the distributed parameter bioreactor in Czeczot (1995).

In majority of cases the value of $r(z,t)$ cannot be directly calculated on the basis of the equation (6) since the values of k_1, $\mu(z,t)$ and $X(z,t)$ are nonmeasurable on-line. Therefore the procedure for estimation of the substrate consumption rate at discrete moments of time has been developed on the basis of the recursive least-squares method (Czeczot, 1997, 1998) and is presented below.

4. Estimation of the substrate consumption rate

Let us rearrange the equation (5) to describe the substrate dynamics at a particular point of the reactor tube z_i:

$$\left.\frac{\partial S(z,t)}{\partial t}\right|_{z=z_i} = -\frac{w(t)}{L}\left.\frac{\partial S(z,t)}{\partial z}\right|_{z=z_i} - r(z_i,t). \tag{7}$$

The derivative of the substrate concentration with respect to time can be approximated by means of the simplest finite difference formula:

$$\left.\frac{\partial S(z,t)}{\partial t}\right|_{z=z_i} \approx \frac{S(z_i,t) - S(z_i,t-T_S)}{T_S} \tag{8}$$

with

It is possible to apply more sophisticated backward finite difference formulas but it is impossible to improve the estimation accuracy in this way and, even in some cases, this can make the accuracy worse (Czeczot, 1997).

Based on the orthogonal collocation method (Villadsen and Michelsen, 1978) the profile of the substrate concentration can be interpolated with application of the Lagrange interpolation polynomial:

$$S(z,t) \approx \sum_{p=0}^{N-1} F_p(z) S(z_p,t); \text{ with } F_p(z) = \frac{\prod_{k=0,\,k\neq p}^{N-1}(z - z_k)}{\prod_{k=0,\,k\neq p}^{N-1}(z_p - z_k)}. \tag{9}$$

As it is known for the orthogonal collocation method, for N points of collocation z_p $(p = 0, \ldots, N-1)$ the boundary points are chosen as $z_0 = 0$, $z_{N-1} = 1$ and the internal points are the roots of the orthogonal Jacobi polynomial. The coefficients of this Jacobi polynomial, and thereby the location of the internal collocation points, depend on the values of two constant parameters $\alpha_K > -1$, $\beta_K > -1$.

On the basis of the expression (9) the approximation of the derivative of the substrate concentration with respect to the space variable at a point z_i can be expressed as follows:

$$\left.\frac{\partial S(z,t)}{\partial z}\right|_{z=z_i} \approx \sum_{p=0}^{N-1} \left.\frac{dF_p(z)}{dz}\right|_{z=z_i} S(z_p,t) = \sum_{p=0}^{N-1} f_{i,p} S(z_p,t). \tag{10}$$

After substituting the expressions (8) and (10) into the equation (7) we can obtain the following equation:

$$S(z_i,t) - S(z_i,t-T_S) = -T_S \frac{w(t)}{L} \sum_{p=0}^{N-1} f_{i,p} S(z_p,t) - T_S r(z_i,t). \tag{11}$$

Let us rewrite the equation (11) in the following way:

$$y(z_i,t) = -T_S r(z_i,t) \tag{12}$$

with

$$y(z_i,t) = S(z_i,t) - S(z_i,t-T_S) + T_S \frac{w(t)}{L} \sum_{p=0}^{N-1} f_{i,p} S(z_p,t). \tag{13}$$

For the above equations it is possible to apply the recursive least-squares method to estimate the value of the substrate consumption rate $r(z_i,t)$ at discrete moments of time:

$$\widehat{r}(z_i,t) = \widehat{r}(z_i,t-T_S) - P(t)T_S(y(z_i,t) + T_S\widehat{r}(z_i,t-T_S)) \tag{14}$$

$$P(t) = \frac{P(t-T_S)}{\cdots}\left(1 - \frac{P(t-T_S)T_S^2}{\cdots}\right) \tag{15}$$

with

α_f — forgetting factor.

Let us note that it is possible to estimate the substrate consumption rate $\widehat{r}(z_i, t)$ at a particular point z_i and at discrete moments of time only if it is possible to access the substrate concentration measurement data at collocation points z_p by means of N substrate concentration sensors. This sensor location allows us to combine relatively small number of sensors, which minimizes the costs of the application, with high accuracy of approximation. Afterwards, we can obtain values of the substrate consumption rate $\widehat{r}(z_p, t)$ at collocation points. It allows us to interpolate the profile of the substrate consumption rate along the reactor tube $\widehat{r}(z, t)$ with application of the Lagrange interpolation polynomial:

$$\widehat{r}(z,t) = \sum_{p=0}^{N-1} F_p(z)\widehat{r}(z_p,t). \tag{16}$$

5. Application of interpolated profile of substrate consumption rate to reactor monitoring

As it was said before, in the case of industrial bioreactors working as wastewater purification biofilters, the total mass of the substrate (organic waste), being reacted due to the biological reaction taking place, is a very important parameter characterizing the biodegradation process. The optimal operating of these units consists in consuming as much of substrate as it is possible under current technological conditions. In this paper the procedure for monitoring of the bioreactor activity is proposed on the basis of the interpolated profile of the substrate consumption rate.

First, let us propose how to calculate the values of two important quantities, characterizing the bioreactor activity, with application of the profile of the substrate consumption rate along the reactor tube $r(z, t)$:

- current mass flux of the substrate being reacted in the reactor tube $M_c^*(t)$ [g/h]

$$M_c^*(t) = \int_V r(z,t)\,dV = AL\int_0^1 r(z,t)\,dz \tag{17}$$

  with

  A [m^2] — cross section of the reactor tube.
- total mass of the substrate reacted in the reactor tube during time T of its activity $M_c(T)$ [g]

$$M_c(T) = \int^{t+T} M_c^*(t)\,dt = AL\int^{t+T}\int^1 r(z,t)\,dz\,dt. \tag{18}$$

Now, on the basis of the above equations, we can apply the interpolated profile of the substrate consumption rate $\widehat{r}(z,t)$ instead of its "true", unknown shape. It allows us to rearrange the formulas (17) and (18) in the following way:

$$\widehat{M}_c^*(t) = AL \int_0^1 \widehat{r}(z,t)\,dz \tag{19}$$

$$\widehat{M}_c(T) = AL \int_t^{t+T} \int_0^1 \widehat{r}(z,t)\,dz\,dt. \tag{20}$$

Since the interpolated profile of the substrate consumption rate $\widehat{r}(z,t)$ is calculated at discrete moments of time, the formula (20) must be written in discrete form to be useful for calculations:

$$\widehat{M}_c(t) = \widehat{M}_c(t - T_S) + T_S AL \int_0^1 \widehat{r}(z,t)\,dz. \tag{21}$$

The expressions (19) and (21) represent the most suitable form and were used during simulation runs.

6. Simulation results and concluding remarks

In order to carry out the simulation experiments there is a need to apply a semi-discretization technique, which results in approximation of the original PDE system (1)–(3) by an ordinary differential equation (ODE) model. In this paper the method of orthogonal collocation (Villadsen and Michelsen, 1978; Dochain et al., 1992; Tali-Maamar et al., 1993) has been applied for this purpose. Other methods of PDE systems semi-discretisation can be found in Carver and Hinds (1978), Schiesser (1991), Metzger (1994, 2000).

For the simulation runs the number of collocation points was chosen as $N = 7$ and the parameters of the orthogonal Jacobi polynomial as $\alpha_k = 0$ and $\beta_k = 4$. The parameters of the mathematical model (1)–(4) were chosen in the following way: $\mu_{\max} = 0.35$, $K_C = 0.4$, $k_1 = 1.5$, $k_d = 0.05$, $L = 1$, $A = 0.01$. In the steady state the inlet substrate concentration $S_{\text{in}} = 5$ and the velocity of the flowing medium $w = 0.5$ were assumed. The value of $P = 1000$ and of the forgetting factor $\alpha_f = 0.1$ were taken. The initial profile of the estimated values of the substrate consumption rate $\widehat{r}(z_i, 0) = 1.99$ $(i = 0, \ldots, N-1)$. Estimation of the substrate consumption rate and calculation of both quantities $M^*(t)$ and $M_c(T)$ are carried out with the same sampling time $T_s = 18$ [min].

As it was said before, it is possible to calculate the values of the important parameters needed for monitoring of the bioreactor and defined in Section 5 on the basis of the values of the substrate consumption rate $\widehat{r}(z_i,t)$ that are estimated at the collocation points z_i. Substrate concentration sensors, located at these points, provide information about current substrate concentration $S(z_i,t)$, Let us also note that it is possible to calculate the "true" theoretical profile of the substrate consumption rate along the bioreactor tube $r(z,t)$ by means of the following expression:

$$r(z,t) = \sum_{p=0}^{N-1} F_p(z) r(z_p,t) = \sum_{p=0}^{N-1} F_p(z) k_1 \mu(z_p,t) X(z_p,t). \tag{22}$$

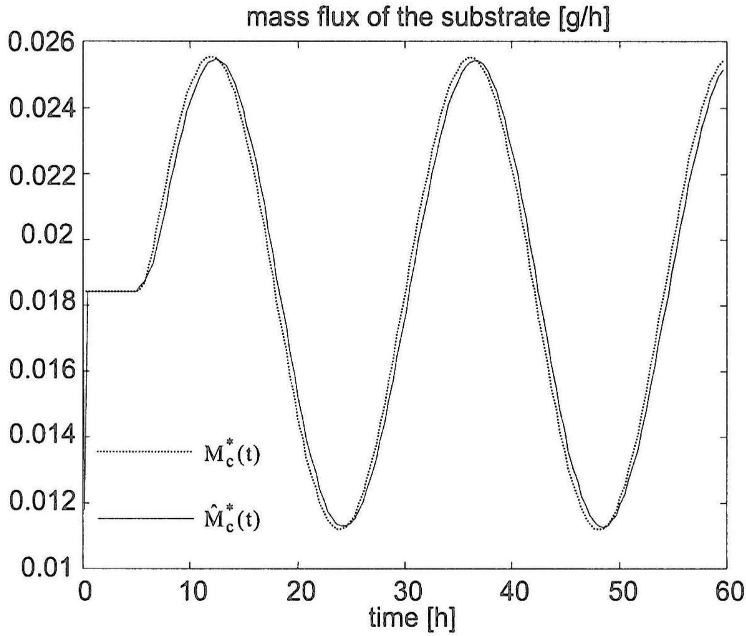
It must be said that the initial values of the substrate consumption rate $\widehat{r}(z_i,0)$ at each collocation point z_i were chosen experimentally to ensure the highest possible estimation accuracy. However, since it is chosen that all the values of $\widehat{r}(z_i,0)$ are equal, while the real shape of $r(z,0)$ has the exponential form, an inaccuracy in the calculation of both quantities $\widehat{M}_c^*(t)$ and $\widehat{M}_c(T)$ follows. This can be seen particularly in the first stage of calculation of the value of $\widehat{M}_c^*(t)$ in the presence of disturbances. It can be noticed that the overregulation arises due to the choice of the initial values of $\widehat{r}(z_i,0)$.

Figs. 1 through 6 present selected simulation results of the values of $M_c^*(t)$ and $M_c(t)$ calculated on the basis of the estimated profile of the substrate consumption rate $\widehat{r}(z,t)$ and in the presence of disturbances. The "true" values of these parameters are plotted with dotted lines and their estimated values with solid lines.

Let us note the very good convergence of the approximated values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ to their "true" values in the presence of the sinusoidal, 24-hour changes (Figs. 1–3) as well as in the presence of the step changes (Figs. 4–6) of the disturbing inlet parameters, namely $S_{\text{in}}(t)$, $w(t)$ and $\mu_{\max}(t)$. This allows us to expect very good monitoring accuracy that ensures not only tracking of the values of the calculated quantities, describing the intensity of the biological reaction taking place inside the bioreactor. It can also provide the possibility to derive the optimal control strategy that is the subject of future work.

The sinusoidal and step changes of the disturbing inlet parameters, applied to the system during simulation runs, are the most commonly used testing signals that are considered at every verification stage. However, these changes have also their physical meaning. The sinusoidal changes of $S_{\text{in}}(t)$ and $w(t)$ correspond to the 24-hour load variations while the $\mu_{\max}(t)$ changes correspond to the 24-hour temperature changes in the case of a biofilter working as a part of a water purification system. If there is a necessity to investigate the influence of such parameters as temperature, pH, dissolved oxygen concentration etc., then the mathematical model of the system has to include state equations for these parameters. Moreover, expression (4) has to have a more complicated form due to the effect of the influence of these parameters on the value of the maximum growth rate $\mu_{\max}(t)$.

The most important implication from this work is the possibility to calculate the values of the substrate current mass flux being reacted in the reactor tube and of the total mass of the substrate reacted during the bioreactor activ-



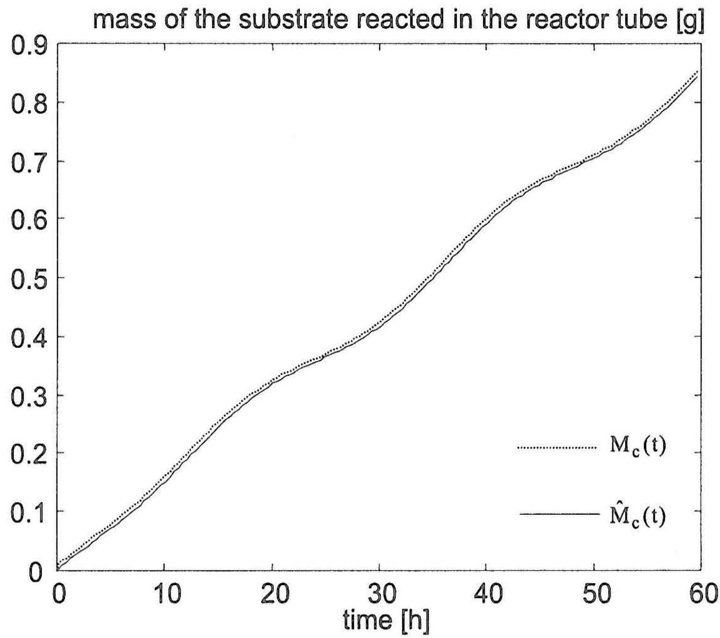


Figure 1. Simulation results of the estimation of the values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ in the

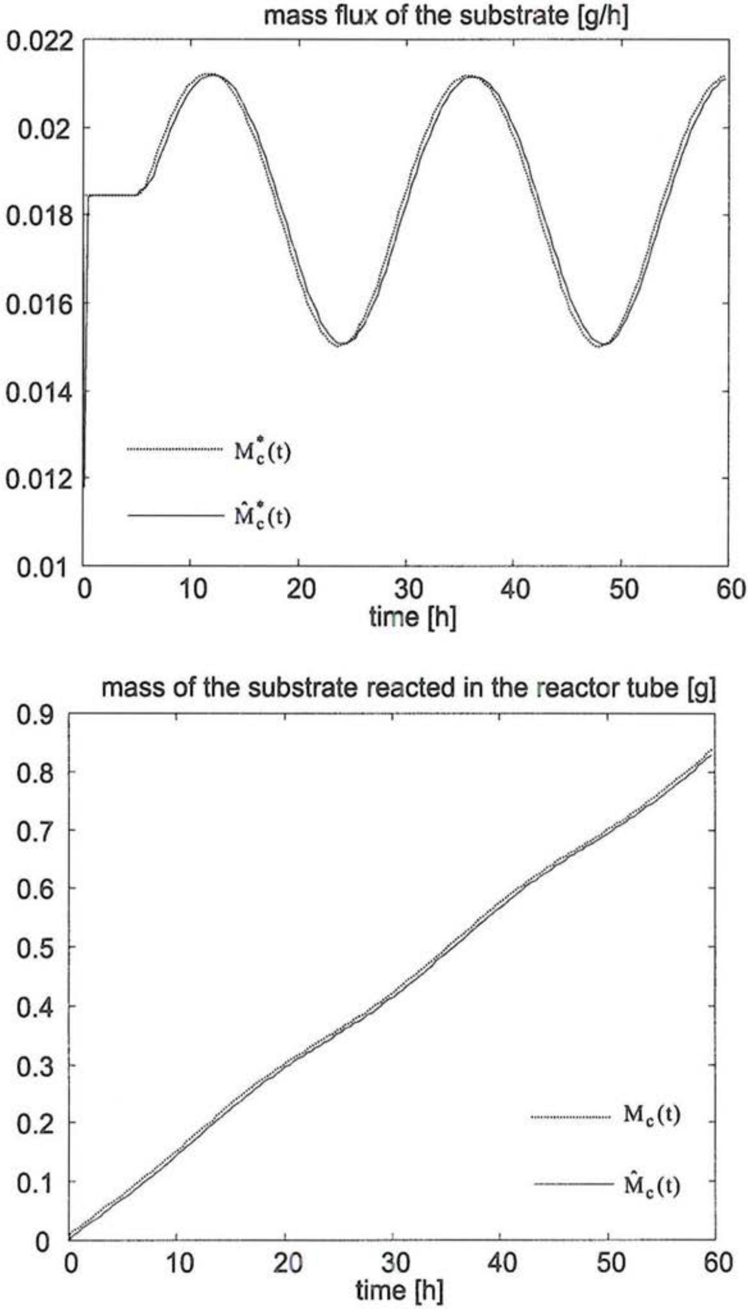


Figure 2. Simulation results of the estimation of the values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ in the

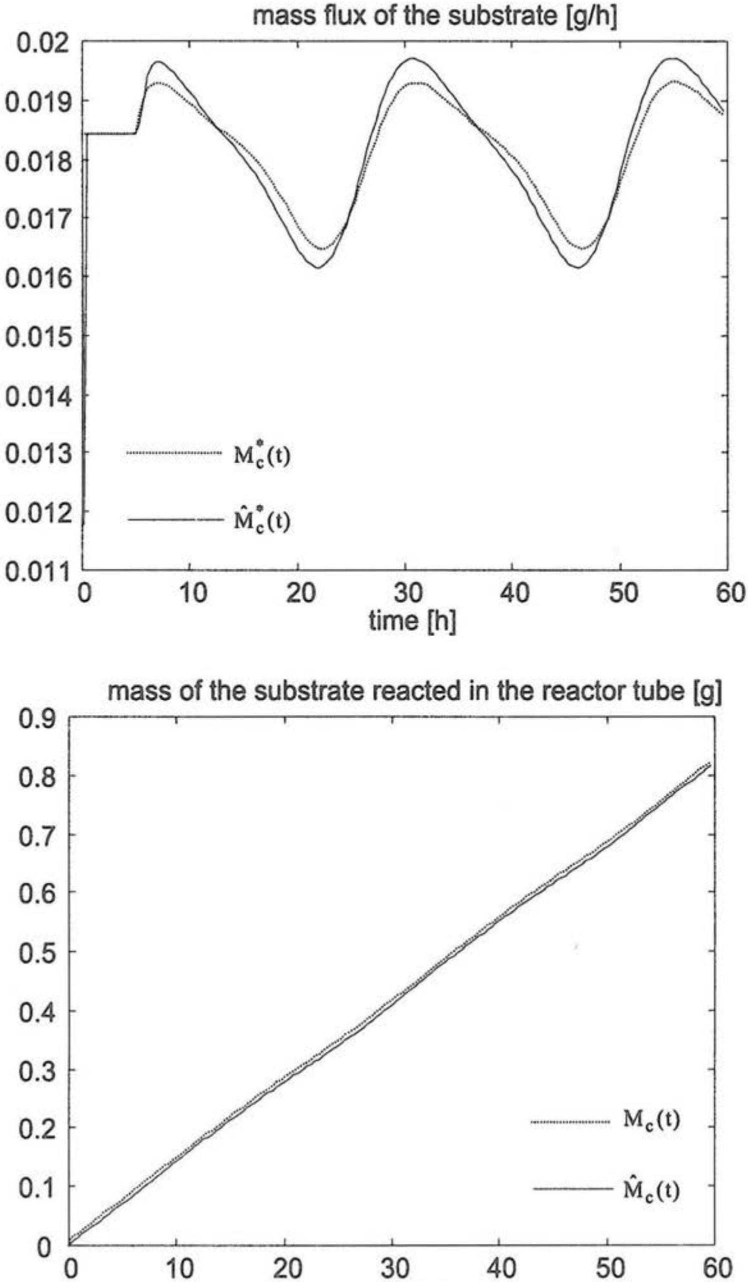


Figure 3. Simulation results of the estimation of the values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ in the

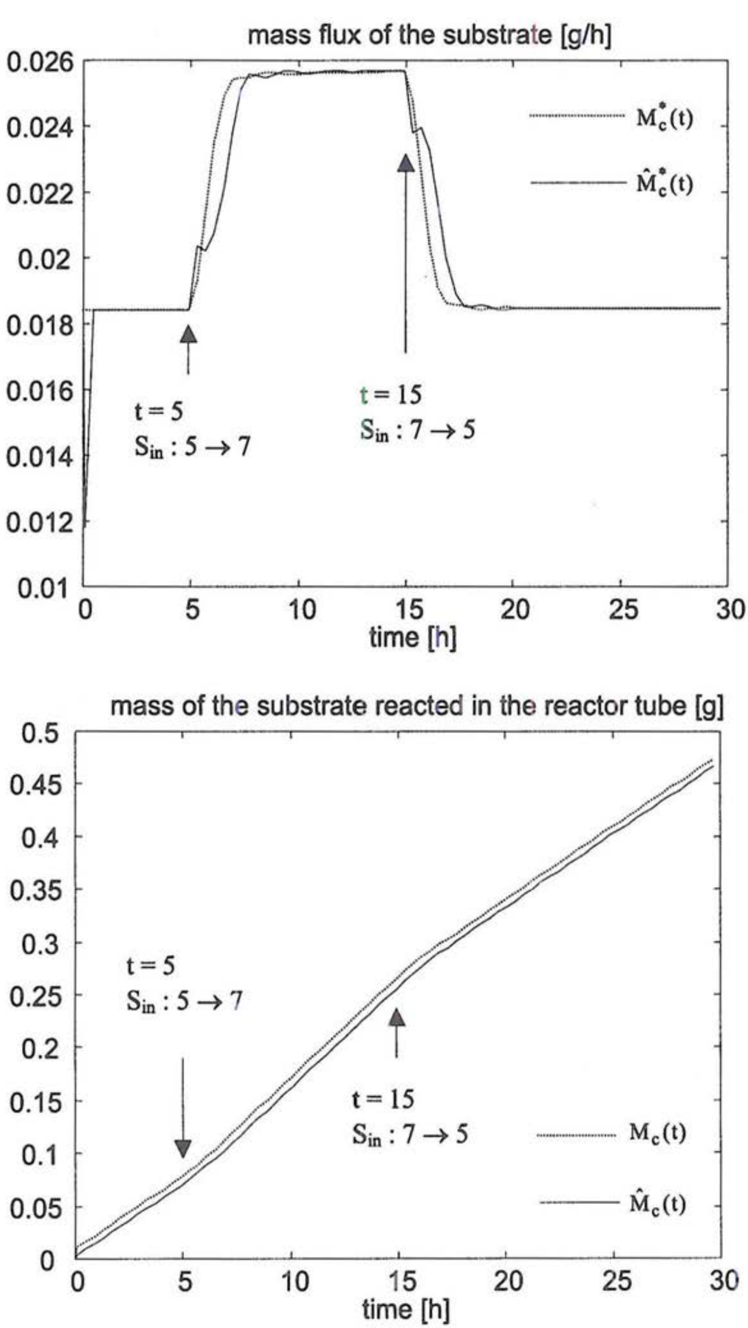


Figure 4. Simulation results of the estimation of the values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ in the

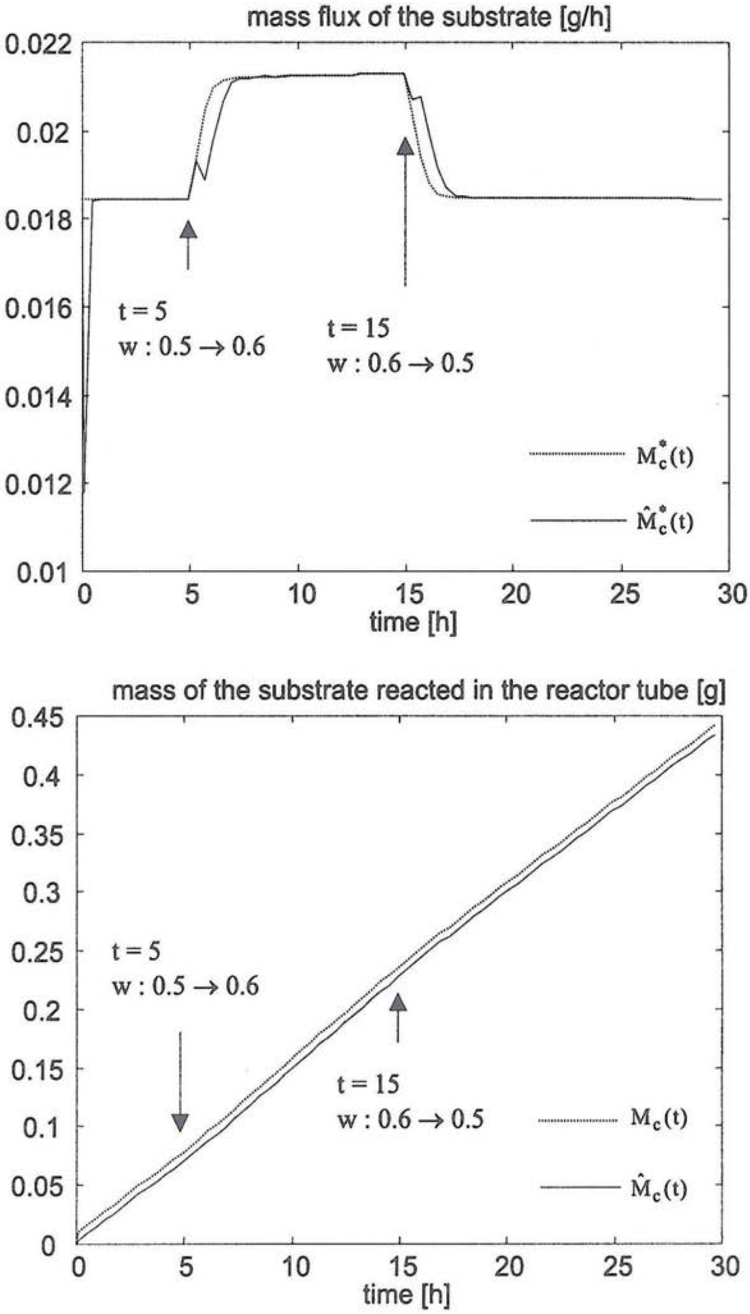


Figure 5. Simulation results of the estimation of the values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ in the

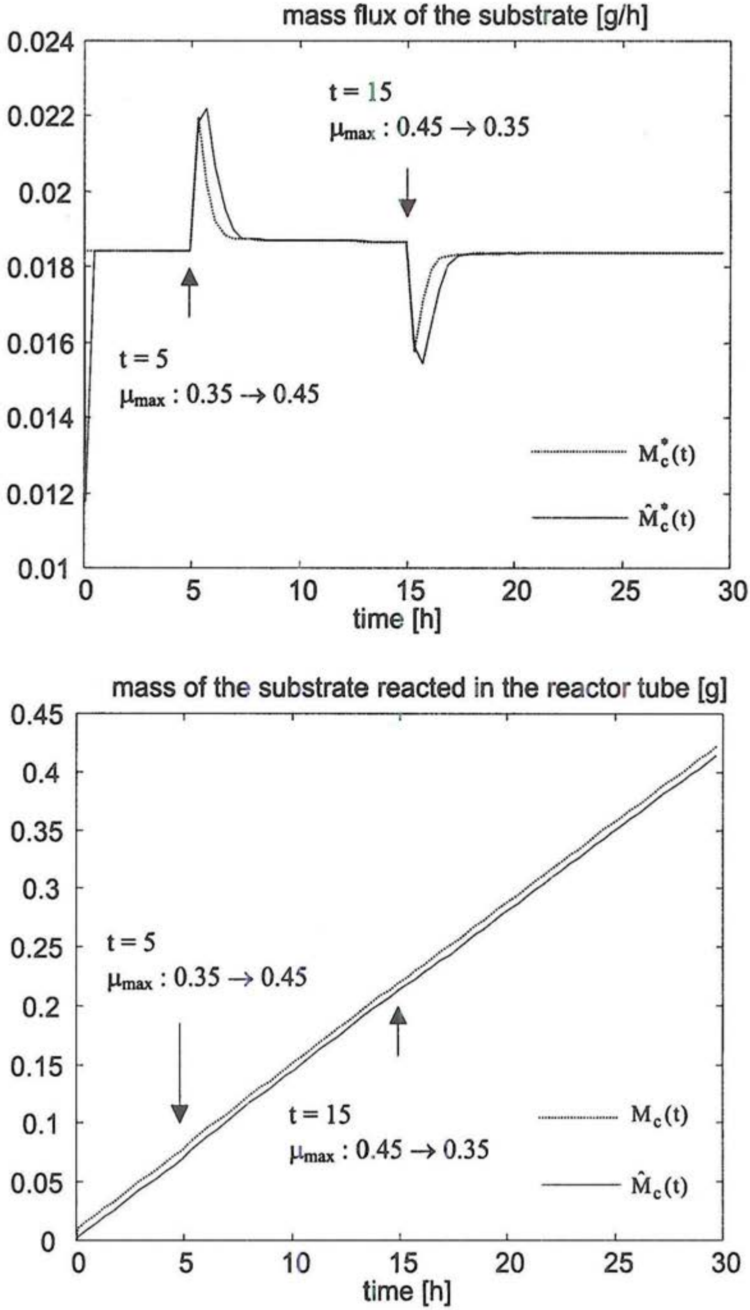


Figure 6. Simulation results of the estimation of the values of $\widehat{M}_c^*(t)$ and $\widehat{M}_c(t)$ in the

intensity of the biological reaction as well as the behavior of every industrial bioreactor applied as a part of a water purification system.

Let us note that the monitoring methodology has been derived on the basis of the substrate consumption rate estimation. The idea of the estimation of this non-measurable parameter is also shown in the paper and has been derived with application of the well known recursive least-squares method. This method allows us to decrease the influence of the measurement noise by adjusting the value of the forgetting factor.

As it was said before in the paper, application of the estimation procedure is followed by the problem of choice of the initial values of the substrate consumption rate at the collocation points. In the here presented work this problem has been managed by comparing the calculated and the "true" theoretical values of the parameters, needed for monitoring of the bioreactor activity, for different initial values. However, such an approach can be used only in the case of simulation experiments since in the practice the "true" values of the calculated parameters are unknown. In order to avoid this problem let us suggest the following idea: why not start the calculations of the parameters, needed for monitoring of the bioreactor, after the first stage of the substrate consumption rate estimation has been carried out? This approach allows us to avoid the problem of the influence of the initial values, chosen for estimation, on the monitoring accuracy.

Some comments should be given on the problem of accessibility of the on-line substrate concentration measurement data in the practical applications. Although the substrate concentration can be determined indirectly on the basis of the COD (chemical oxygen demand) or BOD (biological oxygen demand) measurements, this methodology is very expensive and complicated to be useful in practice. An alternative way to obtain the substrate concentration data consists in deriving the monitoring methodology on the basis of the consumption of the dissolved oxygen due to the biological reaction taking place (respiration rate measurements). This idea has been widely discussed in the literature during the last several years (Kessler and Star Nichols, 1935; Spanjers et al., 1993, 1997, 1998) but it must be said that the access to the on-line respiration rate measurement data still does not ensure satisfying monitoring properties.

In this paper the polynomial interpolation is used because it leads to quite simple solution of the considered problem. The simplicity itself is thus considered as one of the most important features of the suggested methodology and therefore the other possibilities were not taken into account as resulting in more complicated formulation. However, it is interesting to concentrate on the other approximating methods as one of directions for further studies.

To summarize, the methodology, presented in this work, is very general and therefore can be easily applied to any industrial bioreactor or biofilter. This methodology itself bases on the very general form of the mathematical model system nor the values of the physical parameters such as $\mu_{\max}$, K_c etc. It enables successful monitoring, even in the case of strong perturbations from the disturbances or from the parameter uncertainty.

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