MATHEMATICAL MODELLING OF EXTERNAL LOOP FERMENTORS

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ABSTRACT

A comparison between one and the two-dimensional model of external-loop bioreactors is presented. For the models the following assumptions were used: the gas phase is the dispersed phase distributed as gas bubbles in the liquid, radial gradients are neglected; gas hold-up was supposed to be constant; the oxygen distribution in gas bubbles was not accounted for (in one-dimensional model), as well as bubbles size distribution. The models are, non-stationer, dispersed, two-phase, convective. The Houghton approach for liquid extraction was used for the description. It accounts for the oxygen concentration not only in the fermentor (riser and down-comer) but also for the radial concentration profiles in the gas bubbles for the case of two-dimensional model. In the liquid phase the model accounts for oxygen concentration, biomass concentration and substrate concentration being limiting for the microorganisms growth. The kinetics of the biomass growth and the substrate consumption was also calculated. The comparison of the models was done for the oxygen concentration profiles in the gas and liquid phase. In the liquid phase for both models a maximum is observed, more expressed for one-dimensional model. It is to notice that for the case of the one-dimensional model the curves are steeper and the phase saturation values are reached for shorter period. The possible explanation of this fact is the existence of supplementary diffusion resistance in the bubble. The created models can be used for air-lift bioreactors calculations. Possible development of the models is the use of real fermentation media non-Newtonian models.

Keywords: air-lift bioreactor modeling, one- and two-dimensional models – comparison.

INTRODUCTION

In modern technologies as biotechnology the computer control of bioconversion in real time is used. To make possible an effective work of such system the choice of adequate mathematic model of the process is of crucial importance. That is the reason for hard work in this field [3-11, 15, 17]. The aim of the present work is to propose and to compare two mathematical models describing the external loop airlift bioreactor dynamics. In the literature there exist two basic types of bioreactor models: stepwise models [2, 6]: continuous models [6, 8,12], the most detailed of them is the model of K. Leinstrener [6]. The main disadvantage of these models is not accounting for the oxygen concentration distribution in the bubbles as well as the bubble size distribution. That was the reason for us to use the Hutton’s approach for liquid extraction in external loop airlift bioreactor modelling. The same author proposes except the classic dispersed model for liquid extraction, a convective model accounting for dissolved component distribution in the drop and the drops size distribution [1]. In convective model one liquid is treated as a continuous phase, another one – as a dispersed phase. On the other hand the dispersed phase is characterized by the drop size distribution related to drop
velocities distribution and the external mass transfer coefficients from the drops. The drops are supposed to be spherical without liquid circulation. That means that the internal transfer is due only to molecular diffusion. The solution of the equation set for the transfer of the dissolved component in the two-phase composition is possible only for the case when the medium is supposed to be pseudo continuous that means that both phases are treated as existing together in each reactor point. All radial changes are ignored. Only the axial dispersion is accounted for.

**EXPERIMENTAL**

The advantages of external loop airlift bioreactors are: the lack of moving parts, low shear stresses, simplicity of construction, good contact between the phases, long enough residence time of the phases; simplicity in assuring sterile conditions of work. These advantages make it suitable for operation with aerobic microorganisms highly sensitive to shear stresses. The construction of external loop airlift bioreactor is presented below. It consists of riser (1), downcomer (2), gas distributor (3) and gas outlet orifice (4). The gas is introduced in the bottom of the riser through the distributor as bubbles. So in the riser a two phase gas liquid system is formed. Its density is quite lower than that of the pure liquid in the loop.

Because of that it begins a circulation of the fluid in the reactor with upward movement of the gas-liquid mixture in the riser. After separation of the phases in the upper part of the reactor the pure liquid flows down through the loop to the bottom and the process repeats. The gas lives the airlift through the outlet (4). Following this scheme the work of the reactor could be described by a mathematical model consisting of two parts: I – riser and second – downcomer, including the two stages of its work.

First stage: loading of the fermentor. During this stage the liquid phase is saturated with oxygen in absence of biomass and substrate.

Biomass accumulation is the second stage of the process. At the beginning of this stage, accounted by the initial conditions of the model in the liquid phase, saturated with oxygen on the first stage, the biomass and substrate are added. Here the substrate quantity is maximal.

![Diagram](image)

Fig. 1. Air-lift bioreactor: riser (1), downcomer (2), gas distributor (3); gas outlet orifice (4).

The model describing the processes on this stage is similar to that for the first stage, but here the fermentation kinetics must also be accounted for. For its description we chose the Monod equation.

**NUMERICAL EXPERIMENTS**

Two models for description of the processes in external-loop airlift bioreactor are proposed in our work: one- and two-dimensional.

One-dimensional model is unsteady-state, two-phase, dispersion. For simplicity the radial gradients are neglected; gas hold-up was supposed to be constant; the oxygen distribution in gas bubbles was not accounted for, as well as bubbles size distribution.

**Mass balance for the riser**

- Oxygen balance in the gas phase

<table>
<thead>
<tr>
<th>Oxygen concentration change in the reference volume for unity of time</th>
<th>Oxygen rate at the inlet of the reference volume with the gas flow</th>
<th>Oxygen rate at the outlet of the reference volume with the gas flow</th>
<th>Oxygen dissolved in the liquid</th>
</tr>
</thead>
</table>

Based on this balance we can write the following differential equation for the oxygen concentration in the gas phase:
\[
\frac{\partial C_g}{\partial t} + V_g \frac{\partial C_g}{\partial z} - D_g \frac{\partial^2 C_g}{\partial z^2} = -\frac{K_{\text{LA}}}{R_g} \left[ \frac{C_g}{H} - C_{g,1} \right]
\]

(1)

Here \( C_g \) - oxygen concentration in the gas, kg \( \text{m}^3 \), \( C_{g,1} \) - oxygen concentration in liquid, kg \( \text{m}^3 \), \( D_g \) - coefficient of the molecular diffusion, \( \text{m}^2 \text{s}^{-1} \), \( H \) - Henry's constant, \( R_g \) - gas hold-up, \( t \) - time, s, \( V_g \) - gas velocity, \( \text{m} \cdot \text{s}^{-1} \), \( z \) - linear dimension, m.

The appropriate boundary conditions are:

B.C. in the lower part of the riser: \( Z = 0 \)
\( C_g = C_{g,0} \) for the I and II stage
B.C. for the upper part of the riser: \( Z = L_R \)
\( \frac{\partial C_g}{\partial z} = 0 \) for the I and II stage

where \( C_{g,0} \) - max. oxygen concentration in the gas, kg \( \text{m}^3 \), \( L \) - length, m.

- Oxygen balance in the liquid phase

\[
\text{Oxygen concentration change in the phase in the reference volume for entry of time} \quad \text{Oxygen rate at the inlet of the reference volume with the liquid flow} \quad \text{Oxygen rate at the outlet of the reference volume with the liquid flow} \quad \text{Oxygen dissolved in the liquid} \quad \text{Oxygen consumed in the reference volume by the microorganisms}
\]

From this mass balance the following differential equation in partial derivatives can be written for the oxygen balance in the liquid phase:

\[
\frac{\partial C_{c,1}}{\partial t} + V_{c,1} \frac{\partial C_{c,1}}{\partial z} - D_{c,1} \frac{\partial^2 C_{c,1}}{\partial z^2} = -\frac{K_{\text{LA}}}{R_{c,1}} \left[ \frac{C_{c,1}}{H} - C_{c,1} \right] - \frac{1}{Y_{\text{ox}}M_{\text{ox}}} \frac{r_{c,1}}{r_{c,1}}
\]

(2)

Here \( D_{c,1} \) - coefficient of the molecular diffusion in liquid, \( \text{m}^2 \text{s}^{-1} \), \( K_{\text{LA}} \) - transfer coefficient, \( M \) - constant in Monod equation, \( R_{c,1} \) - liquid hold-up, \( Y \) - yield coefficient. The boundary conditions are:

B. C. in the lower part of the riser:
\( Z = 0 \)
\( C_{c,1} = C_{c,1} \)
(for the I stage)
\( Z = 0 \)
\( C_{c,1} = C_{c,2} \)
(for the II stage)

B. C. for the upper part of the riser: \( \frac{\partial C_{c,1}}{\partial z} = 0 \)

for the I and II stage

- Biomass balance

\[
\text{Rate of biomass accumulation in the liquid phase in the reference volume} \quad \text{Biomass rate entering the reference volume with the liquid flow} \quad \text{Biomass rate leaving the reference volume with the liquid flow} \quad \text{Net rate of the biomass generation in the reference volume}
\]

As a consequence the differential equation for the biomass in the liquid phase has the following form for the first zone:

\[
\frac{\partial B_{c,1}}{\partial t} + V_{c,1} \frac{\partial B_{c,1}}{\partial z} - D_{c,1} \frac{\partial^2 B_{c,1}}{\partial z^2} = r_{b,1}
\]

(3)

where \( B \) is the biomass concentration, kg \( \text{m}^3 \)

Boundary conditions:

a) \( Z = 0 \)
\( \frac{\partial B_{c,1}}{\partial z} = B_1 = B_2 \)

b) \( Z = L_r \)
\( \frac{\partial B_{c,1}}{\partial z} = 0 \)

- Substrate balance

The differential equation and the boundary conditions for this balance are, as follows:

\[
\frac{\partial S}{\partial t} + V_{c,1} \frac{\partial S}{\partial z} - D_{c,1} \frac{\partial^2 S}{\partial z^2} = \frac{1}{Y_{\text{ox}}M_{\text{ox}}} r_{s,1}
\]

(4)

Here \( S \) - substrate concentration, kg \( \text{m}^3 \), \( r \), \( R \) - radii, m

B.C.: \( z = 0 \)
\( \frac{\partial S}{\partial z} = S_1 = S_2 \)
\( Z = L_r \)
\( \frac{\partial S}{\partial z} = 0 \)

Mass balances in the loop

In the downcomer there is no gas phase, so only the balances for the liquid phase are to be done:

Oxygen balance in the liquid phase:

\[
\frac{\partial C_{c,2}}{\partial t} + V_{c,2} \frac{\partial C_{c,2}}{\partial z} - D_{c,2} \frac{\partial^2 C_{c,2}}{\partial z^2} = \frac{C_{c,2}}{Y_{\text{ox}}M_{\text{ox}}} \frac{r_{b,2}}{r_{b,2}}
\]

(5)

B. C.
\( Z = 0 \)
\( C_{c,2} = C_{c,1} \)
\( Z = L_r \)
\( \frac{\partial C_{c,2}}{\partial z} = 0 \)

Biomass balance:

\[
\frac{\partial B_{c,2}}{\partial t} + V_{c,2} \frac{\partial B_{c,2}}{\partial z} - D_{c,2} \frac{\partial^2 B_{c,2}}{\partial z^2} = r_{b,2}
\]

(6)

B.C.
\( Z = 0 \)
\( B_{c,2} = B_{c,1} \)
\( Z = L_r \)

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Substrate balance:
\[
\frac{\partial S_g}{\partial t} + V_c \frac{\partial S^2_g}{\partial z} - D_c \frac{\partial S^2_g}{\partial z^2} = -r_{S,g} \quad (7)
\]

B. C. \quad Z = 0 \quad S_g = S_i

B) \quad Z = L_r \quad \frac{\partial S_g}{\partial z} = 0

Two-dimensional model
For two-dimensional model the Hatton approach for liquid extraction was used [1]. Two-dimensional model is two-phase, convective, unsteady-state. The following simplifications are applied: the radial gradients are neglected; gas hold-up in the riser was supposed to be constant; the two-phase system is treated as pseudo homogeneous, i.e. the both phases exist together in each point of the riser and the bubbles are treated as points with their own volume and mass. The gas phase is dispersed and distributed in the continuous liquid phase in the form of bubbles. There is no internal circulation in the bubbles, so the mass transfer in them is conducted only by molecular diffusion; the bubbles size distribution was not accounted for – they are supposed to be with uniform size.

Mass balance for the riser
The oxygen balance in the gas phase is expressed by the equation:
\[
\frac{\partial C_g}{\partial t} + V_g \frac{\partial C_g}{\partial z} - D_g \frac{\partial^2 C_g}{\partial z^2} = -D_g \frac{\partial}{\partial r} \left( r^2 \frac{\partial C_g}{\partial r} \right) \quad (8)
\]

The right side of the equation accounts for the oxygen distribution in the bubble Boundary conditions:

A) \quad Z = 0 \quad C_g = C_{g,0} \quad \text{(for I and II stage)}

B) \quad Z = L_r \quad \frac{\partial C_g}{\partial z} = 0 \quad \text{(for I and II stage)}

C) \quad r = 0 \quad \frac{\partial C_g}{\partial r} = 0 \quad \text{(for I and II stage)}

D) \quad r = R - D_i \frac{\partial C_g}{\partial r} = K_L \left[ \frac{C_g}{H} - C_{g,i} \right]

The oxygen balance in the liquid phase as well as the balances of the biomass and the substrate in the I and the II zone in the two-dimensional model and the boundary conditions are identical to those of the one-dimensional model. The both models were approximated by finite differences method [13, 14, 16] and solved numerically by means of Basic for HP-310.

NUMERICAL RESULTS AND DISCUSSION

The aim of the numerical experiments was to compare both mathematical models and to study in details the two-phase one. The comparison had been made for the both work stages of the airlift fermentor: the preparatory stage, when the liquid phase is saturated with oxygen and the operational stage, characterized by the biomass growth.

In Figs.2.1 and 2.2 the concentration profiles of the oxygen for the riser in the gas and the liquid phase for the one and the two-dimensional models are presented. It is evident that the profiles have similar forms for both models. The oxygen profile for the gas phase decrees continuously to 0 at the beginning of the process. With the time due to the liquid phase saturation with oxygen and decreased driving force (i.e. the flux through the bubble interface) the profile flattens until the constant values along the riser in the end of the first stage. Similar phenomenon is observed for the gas bubble oxygen profiles (see Fig.2.3). At first the decrease of oxygen concentration from the centre to the bubble interface is observed. In the end of the stage the radial profiles reach certain value, after which the oxygen concentration in the bubbles increases with the time.

In the liquid phase for both models a maximum in oxygen concentration is observed, more expressed for one-dimensional model. It is to notice that for the case of the one-dimensional model the curves are steeper and the phase saturation values are reached for shorter period. The possible explanation of this fact is the existence of supplementary diffusion resistance in the bubble.

Similar results were obtained for the second stage of the process which could be seen in Figs 2.4 and 2.5, presenting the concentration profiles in both phases along the riser for one and the two-dimensional model.

Because of the lack of oxygen inhibition effect on the biomass growth, the profiles of the substrate and bio-
Fig. 2. 1. Oxygen concentration profiles of in the gas phase in the riser for the I stage: a - one dimensional model; b – two-dimensional model.

Fig. 2. 2. Oxygen concentration profiles of in the liquid phase in the riser for the I stage: a - one dimensional model; b – two-dimensional model.

Fig. 2. 3. Oxygen concentration profiles in the bubble.

Fig. 2. 4. Oxygen concentration profiles of in the gas phase in the riser for the II stage: a - one dimensional model; b – two-dimensional model.
mass for both models could be calculated independently. As they concern just the liquid phase the results are logically the same for both models.

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