International Journal of Pure and Applied Mathematics
Volume 49 No. 1 2008, 1-12

MASS TRANSFER INVESTIGATIONS IN A BUBBLE COLUMN BIOREACTOR

Dimitrinka Popova[1], Dessislava Moutafchieva[1], Stilijan Tchaoushev[1], Tsolo Tsolov[2] §, Ivan Pentchev

[1]Department of Chemical Engineering
University of Chemical Technology and Metallurgy
Sofia, 1756, BULGARIA
e-mail: dspk07@uctm.edu
[2]Department of Polymer Engineering
University of Chemical Technology and Metallurgy
Sofia, 1756, BULGARIA

Abstract: A two-dimensional unsteady-state dispersion model for two-phase gas-liquid bubble column is presented. The model is developed for prediction of axial concentration profiles of dissolved oxygen in bubble column with and without microorganisms. The solution of the model is obtained by means of finite difference method. Experimental data are used for examination of validility of the model solution.

AMS Subject Classification: —???—
Key Words: dispersion model, bubble column, finite difference method, oxygen concentration profiles

1. Introduction

Bubble columns are widely used in chemical industry as reactors and in biotechnology as fermenters. Their main advantage is a simple construction. They are known as efficient mixers, if only low energy input levels are required. The design and scale-up of bubble column reactors are difficult (although) that's why they have been investigated for many years. Because their fluid dynamics appear to be very complex it is not possible to scale them up from first

Received: March 11, 2008

§Correspondence author

principles.

A bubble column consists of a cylindrical tank with an aspect ratio usually between 2 and 10. At its bottom a gas sparger produces bubbles, and dispersed gas phase moves in a continuous liquid phase.

The most common approach to modeling bubble columns has been based on dispersion models [8]. Two-phase dispersion models were applied for the calculation of bubble columns with and without internal recycle since the end of the 1960s. [2] Dispersion models for bubble columns have been presented for chemical systems by Deckwer, 1976 [3]. An analytical method for design and solution of a bubble column fermenter without pressure has been given by Shioya, Dang and Dunn 1978 [4]. Since 1980s more detailed two-phase models for multidimensional flow simulations were developed and tested.

The model equations used are usually balance equations and are formulated for both phases. Finite volume discretization and iterative solutions mostly based on the SIMPLER algorithm of Patankar [7] have been applied for the numerical solution.

Design of gas-liquid bubble columns has so far mainly been carried out by means of empirical and semi-empirical correlations which have been gained from experimental data e. g. of mass transfer for bubble columns of different scales [18].

The mass transfer characteristics belong to the most important parameters for design and scale up of bubble columns and naturally they have been the subjects of much research. The oxygen transfer is expressed in terms of a constant or inconstant coefficient (gas hold-up, dispersion, velocity) and liquid phase driving force. In the literature many articles discussed this [10, 11, 14].

When the bubble columns have been employed as bioreactors for aerobic microbiological processes the design of such apparatus requires the consideration of substrate concentration and it is assumed that for the bubble column fermenter design the most important is the oxygen concentration gradients.

Sioya and Dunn [5] present two gas-liquid dispersion models for the description of the oxygen concentration profiles in a bubble column fomenter. Model I is obtained from steady state oxygen balance with equations for gas and liquid phases. It is simpler and with analytical solution. Model II includes the effect of hydrostatic pressure gradient on the gas velocity and the oxygen solubility. The model contains equations for total gas balance – gas and liquid oxygen balance.

In the work was used the quasi-linearization method for solving. This method was found to be not generally applicable to the entries parametric range of interest because the solution is highly sensitive to the choice of initial conditions. As of the large number of governing parameters in these models it is not possible to make a model comparison for every simulation.

In the second paper the authors have made dynamic oxygen transfer experiments in bubble column. The model was supplement (added) with a second order lag relation for the electrode. The validity of the solution has been demonstrated using simulation data obtained by numerically integrated the model equations.

The objective of this work is to describe a relevant engineering system modeled by a system of nonlinear parabolic partial differential equations. This description will require the solution of the system of equations using a numerical method. Experimental data will be used to verify the model solutions for desalt water and production of thilozine in a bubble column industrial reactor.

A bubble column reactor (BCR) is a pipe. Reactants are fed in the top of the pipe and some mixture of reactants and products emerge from the bottom. The concentration inside the BCR can vary with time, axial position, radial position, and angular position. For the purposes of this derivation, we are going to assume that the variations in the radial and angular directions are negligible. Therefore, the concentration is only functions of time and axial position. The equations that describe the behavior of a are material and energy balances. We are looking for a solution of material balance equations.

2. Equipment

All measurements were performed in bubble column fermentor with total volume 1300 l and 1000 l work volume, L/d ratio = 2.

Desalt water and tylozin (*streptomyces fradiae*) as a biomass were used as the liquid phase and air as gas phase. A viscometer with coaxial cylinder and six-blade impeller was used for rheological measurements.[14] The oxygen concentration is followed with a P2 – type dissolved oxygen probe and a 703P polarographic oxygen meter from Uniprobe. The probe was located at the 500 mm from the bottom of the column at a 45^0 angle. The dry sell concentration was estimated by calculating the dry weight from the weight of cells per volume of sell suspension. Each measurement of oxygen and biomass concentration was made at interval of 4 hours during the whole fermentation process which

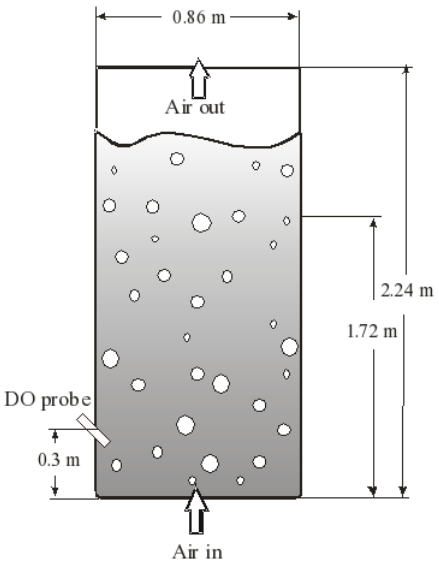

Figure 1: Bubble column experimental set-up

continue 130 hours.

3. The Model

A model is developed for prediction of axial concentration profiles of dissolved oxygen in bubble column contactor with and without microorganisms. Experimental data are used to verify the model solutions for desalt water and production of thilozine in a bubble column reactor with 1 m^3 work volume.

The oxygen is transported (transferred) from the gas phase to the aqueous medium to provide the microorganisms with determined rate. Therefore, modeling of the reactor has to consider gas-liquid mass transfer and hydrodynamics (gas-liquid interfacial area, gas holdup). Whereas dissolved oxygen concentration is function of position along the reactor and basically of time and the model is assumed (given in account) this. The concentration profiles are calculated (estimated) as a function of time (at equal time intervals) or of height of the reactor (at equal length intervals). This is reasonable because a short time changing of oxygen concentration (increment in liquid phase and decrement in gas phase).

The transfer of oxygen from air to the cell during a fermentation process pass over a number of steps [1] (1) the transfer of oxygen from an air bubble into the solution, (2) the transfer of the dissolved oxygen through the fermentation medium to the microbial cell, and (3) the uptake of the dissolved oxygen by the sell. The model for a column reactor can be formulated as a two-phase axial dispersion model. The unsteady-state oxygen balance for a two-phase system with term, accounting for the presents of cells may be written as:

For gas phase:

$$\frac{\partial(\varepsilon_G C_G)}{\partial\tau} + U_G\frac{\partial(\varepsilon_G C_G)}{\partial z} = \frac{\partial}{\partial z}\left(D_G\varepsilon_G\frac{\partial C_G}{\partial z}\right) - K_L a(C_L^* - C_L)\,. \qquad (1)$$

For liquid phase:

$$\frac{\partial(\varepsilon_L C_L)}{\partial\tau} + U_L\frac{\partial(\varepsilon_L C_L)}{\partial z} = \frac{\partial}{\partial z}\left(D_L\varepsilon_L\frac{\partial C_L}{\partial z}\right) - K_L a(C_L^* - C_L) - P\,. \qquad (2)$$

C_L is the continuous phase concentration, C_G is the dispersed phase concentration, and the velocity, dispersion coefficient for each phase and the volumetric mass transfer coefficient are the phenomenological coefficients.

The term P of equation (2) is represented subsistence of microorganisms in the reactor. Oxygen consumption in the fermentor is related to the growth of the microorganisms. The specific growth rate may be represented as (can be described by):

$$P = \begin{cases} \dfrac{\partial C_i}{\partial t} - D_i\dfrac{\partial^2 C_i(z,t)}{\partial z^2} = Q_i(z,t)\,, \\ Q_i = \mu_{\max}\dfrac{C_S}{K_S + C_S}\dfrac{C_0}{K_0 C_X + C_0}\,. \end{cases} \qquad (3)$$

We have needed to employ a numerical method capable of solving a system of coupled, nonlinear, parabolic partial differential equations.

The solution of the model is obtained by means of finite difference method.

We have used implicit finite-difference approximation scheme, which permit an independent choice of the time and space parameters of the gird. [6]

A peculiarity of difference equations is that the matrix of the coefficients has a tridiagonal structure and (we can use successful) one of the most widely used method for solution of such equations is the Gaussian two-step elimination method or factorization procedure.

We started by re-writing the equations 1 and 2 in dimensionless form. For non-dimensionalization of equations we have used the follow scales:

For concentration – c_{Go} (initial oxygen concentration in gas phase); for

length coordinate – L (height of the reactor); for velocity – U_{Go} (initial superficial gas flow velocity); for time – $\dfrac{L}{U_C}$; for oxygen dispersion coefficient – D_{G0} - dispersion coefficient of gas phase;

Non-dimensiolization

$$\bar{C}_G = \frac{C_G}{C_{G0}}\,, \quad \bar{D}_G = \frac{D_G}{D_{G0}}\,, \quad \bar{\tau} = \frac{\tau U_{G0}}{L}\,,$$
$$\bar{C}_L = \frac{C_L}{C_{G0}}\,, \quad \bar{D}_L = \frac{D_L}{D_{G0}}\,, \quad \bar{z} = \frac{z}{L}\,,$$
$$\bar{U}_G = \frac{U_G}{U_{G0}}\,, \quad \bar{B}_0 = \frac{UL}{D}\,,$$
$$\bar{U}_L = \frac{U_L}{U_{G0}}\,.$$

For dimensionless form of the equations (1) and (2) we have obtained:

$$\frac{\partial(\varepsilon_G \bar{C}_G)}{\partial \bar{\tau}} + U_G \frac{\partial(\varepsilon_G \bar{C}_G)}{\partial \bar{z}} = \frac{\partial}{\partial z}\left(\bar{D}_G \varepsilon_G \frac{\partial C_G}{\partial z}\right) - K_L a(\bar{C}_L^* - \bar{C}_L)\,. \qquad (4)$$

$$\frac{\partial(\varepsilon_L \bar{C}_L)}{\partial \bar{\tau}} + U_L \frac{\partial(\varepsilon_L C_L)}{\partial \bar{z}} = \frac{\partial}{B_{0L}\partial \bar{z}}\left(\bar{D}_L \varepsilon_L \frac{\partial C_L}{\partial \bar{z}}\right) - \frac{L}{U_{G0}} k_L a(\bar{C}_L^* - \bar{C}_L) - \frac{L}{U_{G0}} P\,. \qquad (5)$$

The initial conditions are:

$$C_G|_{z=0,\,\tau=0} = C_{G0}\,, \quad C_L|_{z=0,\,\tau=0} = 0\,.$$

The boundary conditions are:

at $z = 0$

$$D_G \frac{\partial C_G}{\partial z}|_{z=0} = U_G(C_{G0} - C_G|_{z=0})\,,$$
$$D_G \frac{\partial C_G}{\partial z}|_{z=L} = D_L \frac{\partial C_L}{\partial z}|_{z=L} = 0\,,$$

at $z = L$

$$D_G \frac{\partial C_G}{\partial z}|_{z=L} = D_L \frac{\partial C_L}{\partial z}|_{z=L} = 0\,.$$

Because of the very small parameter at higher partial derivative the convergence of scheme has disturbed. The scheme becomes unstable (stability is the necessary and sufficient condition for convergence) and it has to required using a special numerical procedure of exponential approximation [9]

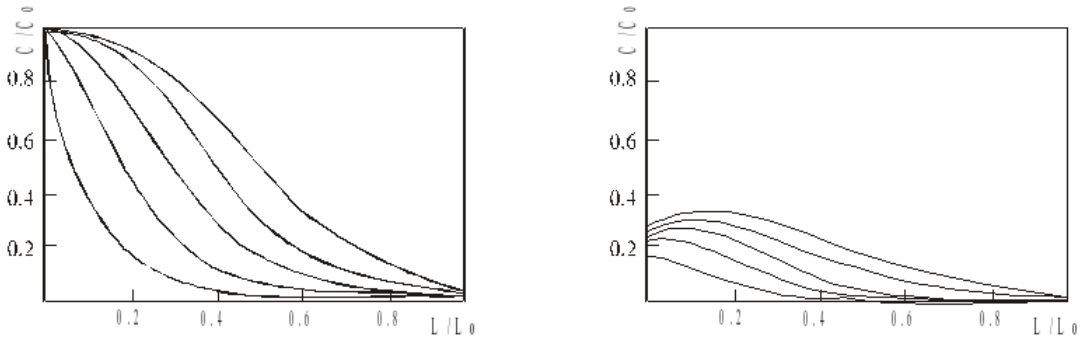

Figure 2: Dimensionless profiles of oxygen concentration in gas and liquid phases along the fermentor – numerical results for five steps in time ($K_{La} = 0,0693$, $L = 10$m, without biomass)

4. Numerical Results

In this section we present the numerical investigations resulting from the solution of the dispersion model. or (of the results obtained by). The correlations used for each of parameters, which appear in the equations, are: $\varepsilon_G = 0.0256U_G^{0.82}$, $D_L = 2.7d_c^{1.4}U_G^{0.3}$.

Figure 2 shows numerically obtained oxygen concentration profiles of gas and liquid phases along the fermenter based on follow assumptions:

1. Radial mixing in the column is perfect;

2. The dispersion coefficient is independent of position;

3. Resistance to mass transfer due only the interaction between the gas and the liquid phases;

4. Unsteady state, turbulent flow.

The values of K_{La}, obtained (received) through experimental data, are estimated by optimization procedure as minimum deviation between experimental data and calculated results. The experiments were carried out by gas and liquid flow rates obtained by method described in our paper [17]

We have made comparison between two phase dispersion model solution obtained by means of finite difference method and the results published by Shioya and Dunn, based on moment analysis.

Figure 3 shows numerically obtained oxygen concentration profiles of gas and liquid phases along the fermenter based on the parameters used by Sioya

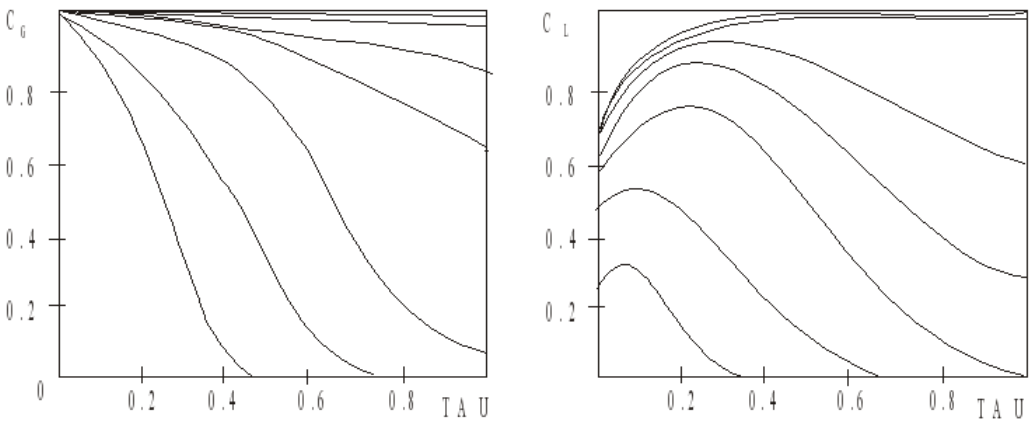

Figure 3: Dimensionless profiles of oxygen concentration in gas and liquid phases along the fermenter in conditions, used by Shioya and Dunn

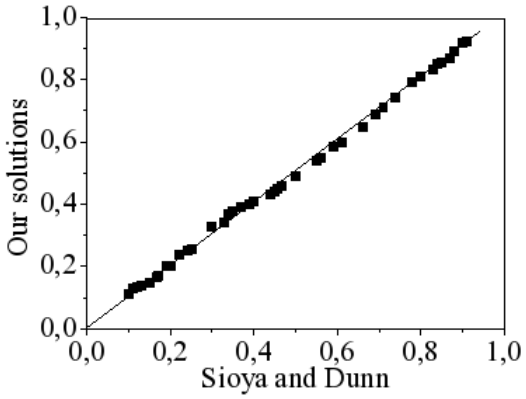

Figure 4: Comparison between the model solutions made by Shioiya and Dunn [4] and by means of finite difference method at equal parameters showed above

and Dunn in his paper [4]:

$$L = 10m\,,\ D_G = 0.04m^2s^{-1}\,,\ C_{L0} = 0\,,\ \varepsilon_G = 0.1\,,$$
$$U_G = 0.2m\,s^{-1}\,,\ D_L = 0,04m^2s^{-1}\,,\ C_{G0} = 1\,,\ \varepsilon_L = 0.9\,,$$
$$U_L = 0.02m\,s^{-1}\,,\ K_La = 0.066s^{-1}\,.$$

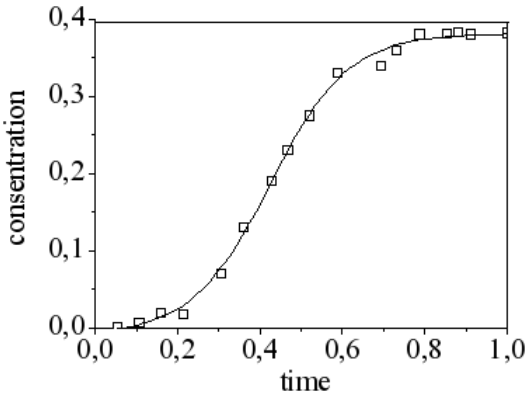

Figure 5: Dimensionless oxygen concentration profile in liquid phase in time ($K_La = 0,0753$, $L = 2m$, without biomass); (—) – the model solution; ([F087?]) – experimental data (desalt water)

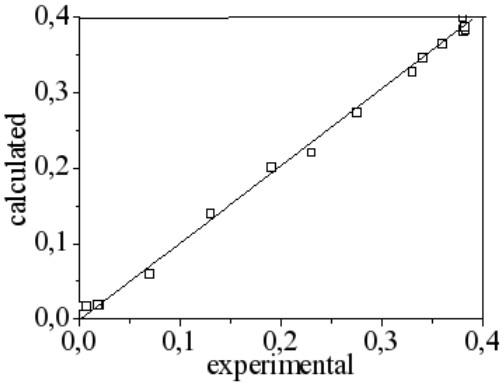

Figure 6: Comparison between the model solution and normalized experimental data. The U_G, U_L and K_La have been estimated as it is referred above

Figure 4 shows the time dependent oxygen concentration profile (points) which develop when the column is initially deoxygenated with nitrogen. As it has shown in Figure 4, the simulations (line) reproduced the measurements the closeness of fit depended on the variable being predicted. Significantly (Generally), in all cases the predicted and the observed qualitative behaviors were quit consistent.

Ideally, the correlation between simulated and experimental data should be

straight line: the parity plot should have zero intercept and unit slope. As it is shown in Figure 5, the normalized (value maximum/value) experimental observations and the simulations generally correlated well. The degree of correlation differs for different variables. The mean of errors for the entire group of variables is lower than 8 %. Obviously, the model is sufficiently reliable of a range of parameters for predicting behavior.

Numerical solutions are validated for a given flow system. They can be easily used for a scientific reactor scale-up. The different bubble size, the different gas spargers and superficial gas velocities on the structure of two phase flow, the influence of aspect ratio and the column geometry can be detailed investigated. This is a subject of our current work.

5. Conclusions

A two dimensional unsteady state two-phase dispersion model was proposed for prediction of axial concentration profiles of dissolved oxygen in bubble column fermenter with and without microorganisms. Experimental data were used to verify the model solutions for desalt water and production of thilozine in a bubble column reactor with 1 m^3 work volume.

The comparison between the results of simulations and experimental data published by Shioya and Dunn [4] and our investigation were made. Coincidence between the models solutions has been found as satisfaction.

It has be made paralel with experimenta data obtained by desalt water and thilozin production. The simulations were closely agreed with the measurements.

Experimental data have been used to demonstrate that the solution of the model and the method of this solution are agrees well with experimental observations.

Nomenclature

Bo	Bodenstein number	[-]
C	oxygen concentration	[kg m^{-3}]
D	oxygen diffusivity	[m^2 s^{-1}
d	diameter	[m]
K	kinetic constant	[-]
K_La	volumetric mass transfer coefficient	[s^{-1}]
L	length of the reactor	[m]
U	velocity	[m s^{-1}]
Q	volumetric reaction rate	[kg m^{-3} s^{-1}]
z	coordinate	[m]
μ	specific growth rate	[s^{-1}]
ε	gas hold-up	[-]
τ	time	[s]
G	gas	
i	component index	
L	length	
O	oxygen	

References

[1] W.H. Bartolomew, E.O. Karrow, M.R. Sfat, R.H. Wilhelm, Oxygen transfers and agitation in submerged fermentations, *Ind. Eng. Chem.*, **42** (1950), 1801-1809.

[2] N. Zuber, J.A. Findlay, Average volumetric concentration in two-phase flow systems, *J. Heat Transfer*, **453** (1965).

[3] W.D. Deckwer, *Chem. Eng. Scs.*, **31**, (1976).

[4] S. Shioya, N.D.P. Dang, I.J. Dunn, Bubble column fermentor modeling: comparison for pressure effect, *Chem. Engng. Sci.*, **33** (1978), 1025.

[5] I.J. Shioya Dunn, A dynamic transfer coefficient measurement method for column reactors, *Chem. Engng. Sci.*, **33** (1978), 1529.

[6] E.F. Nogotov, B.M. Berkovsky, *Applications of Numerical Heat Transfer*, UNESCO, Paris (1978), 16-98.

[7] S.V. Patankar, *Numerical Heat Transfer and Fluid Flow*, McGraw Hill, New York (1980).

[8] W.D. Deckwer, K. Nguen-Tien, A. Shumpe, Y. Serpemen, Oxygen mass transfer into aerated CMC solutions in a bubble column, *Biotechnology and Bioengineering*, **XXIV** (1982), 461.

[9] E.P. Doolan, J.J.H. Miller, W.H.A. Schilders, *Uniform Numerical Methods for Problems with Initial and Boundary Layers*, Mir, Moskow (1983).

[10] M.W. Haque, K.D.P. Nigam, V.K. Srivastava, J.B. Joshi, K. Viswanathan, Studies on mixing time in bubble columns with pseudo plastic CMC solutions, *Ind. Eng. Chem. Res.*, **26** (1987).

[11] M.W. Haque, K.D.P. Nigam, K. Viswanathan, J.B. Joshi, Studies on gas holdup and bubble parameters in bubble columns with CMC solutions, *Ind. Eng. Chem. Res.*, **26** (1987), 86.

[12] D.S. Van Vuuren, The transient response of bubble columns, *Chem. Eng. Sci.*, **43** (1988).

[13] A. Lapin, A. Lübbert, Numerical simulation of dynamics of two-phase gas-liquid flows in bubble columns, *Chem. Engng. Sci.*, **49** (1994).

[14] M. Karsheva, J. Hristov, I. Penchev, V., Lossev, Rheological behavior of fermentation broths in antibiotic industry, *Applied Biochem. and Biotechnol.*, **68** (1997).

[15] K. Schügerl, K.H. Bellgardt, *Bioreaction Engineering: Modeling and Control*, Springer-Verlag, Berlin (2000).

[16] S. Tchaoushev, D. Moutafchieva, D. Popova, I. Penchev, Numerical simulation of mass-transfer characteristics of an external airlift reactor, In: *12-th Romanian International Conference on Chemistry and Chemical Engineering*, September 13-15, Bucharest (2001).

[17] V. Michele, *CFD Modeling and Measurement of Liquid Flow Structure and Phase Hold-Up in Two- and Three Phase Bubble Columns*, Ph.D. Thesis, Gemeinsamen Fakultät für Maschinenbau und Elektrotechnik der Technischen Universität Carolo-Wilhelmina zu Braunschwe, Germany (2002).