BakSIM – An application for control, monitoring and simulation of baker's yeast fermentation process

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Abstract *— This paper describes an experience based on the final project work for the Industrial Electronics Engineering undergraduate course. The main goal is the development of an application for fermentation processes. BakSIM is an application for monitoring, control and simulation of a mini-bioreactor for baker's yeast fermentation, running in open or closed loop mode. It performs data acquisition of the most important system variables: biomass, ethanol, oxygen, glucose and dioxide of carbon, and files writing for future analysis and for future contrast with previous experiences. Different modules were considered: simulation, monitoring and simulation and monitoring running together. The BakSIM application allows not only the comparison of the experimental data with the simulated data as the study of the effectiveness of several numerical methods. One more advantage of this project was its multidisciplinary work, enclosing several areas covered during the undergraduate course, namely Programming, Process Control and Numerical Methods.*

Index Terms — Differential Equations, Process Control, Simulation, Undergraduate Research Experiences.

MOTIVATION

Real processes in biochemical and food industry are, in their vast majority, non-linear MIMO (Multiple Input Multiple Output) systems. Their dynamics and control are difficult to study both for theoretical and practical reasons. In many cases, experiments with real industrial processes are not carried out for economy and safety reasons, and frequently on-line measurements are not available or simply they are too expensive [1].

Living cells of *Saccharomyces cerevisiae*, which form baker's yeast, are predominantly used in bakery and beer industries. Its industrial importance and economical significance, promoted its selection as a case study for the application developed.

BakSIM application (Figure 1) was developed for monitoring, control and simulation of a Mini-Bioreactor running in open or closed loop mode. It performs data acquisition of the most relevant system variables: biomass, ethanol, oxygen, glucose and dioxide of carbon, as well as files writing for future analysis and comparison with previous experiences. Different running modes were considered: simulation, monitoring and simulation and monitoring running in parallel. In this case, BakSIM application allows the comparison between experimental and simulated data. The study of the effectiveness of several numerical methods can also be tested, as different numerical routines are available.

The simulation process requires the integration of a set of non-linear differential equations, for the state variables. A set of algebraic equations, concerning mass transfer relations and kinetics laws, can be considered as part of the system to be solved, defining a differential algebraic equation system.

This project was developed in a discipline in the last year of the Industrial Electronics course of Minho University. It was relevant for its multidisciplinary work, including areas focused during the course, namely Programming, Process Control and Numerical Methods.

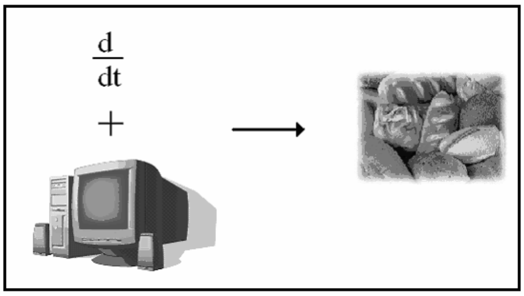

FIGURE. 1
'MAKING BREAD WITH DERIVATIVES AND A COMPUTER'.

BAKER'S YEAST FERMENTATION PROCESS

Baker's yeast production is essentially carried out in a fed-batch fermenter with inoculums of *Saccharomyces cerevisiae* culture and a glucose solution as substrate feed.

The experience and know-how f the team is one of the main reasons for the use of this process in the development of project works for undergraduate course.

Three metabolic pathways characterize the baker's yeast fermentation process, depending on the availability of sugar and/or oxygen: respiratory growth on glucose, fermentative growth on glucose and respirative growth on ethanol.

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Respirative pathways occur in presence of oxygen and the fermentative one in its absence (with production of ethanol) [2]. The metabolic pathways of fermentative growth on glucose and oxidative growth on ethanol are competitive.

This competition is governed by the respiratory capacity of the cells. If the instantaneous oxygen uptake capacity exceeds the oxygen need for total respiratory glucose uptake, then, all sugar uptakes follow the respiratory pathway with the remaining oxygen being spent on ethanol respiratory uptake. Otherwise, if the instantaneous oxygen uptake capacity is not enough, part of glucose uptake follows the respiratory pathway while the remaining follows the fermentative pathway.

Macro system

The macro experimental set-up [3] consists on a five-litre fermenter with temperature control, aeration and agitation. It is equipped with sensors for on-line measurement of environment variables, such as: temperature, pH and concentration of dissolved oxygen. These variables are monitored and controlled by a direct digital control unit (DCU, Biostat MD). Each variable has its own control loop, with appropriate parameters, which can be modified by the user or through the supervisor computer. The controller actuates in each final control element, as for example, acid and base pumps for pH control.

The fed-batch fermentation starts with a 2l volume substrate medium and an inoculum of 0.5l. Substrate addition, dictated by a control law, is monitored with the help of a balance, by means of mass variation of the glass that contains the glucose solution. The feeding ends when the maximum volume is attained (the fermentation time is about 15 to 20 hours).

The knowledge of liquid phase composition, in terms of state variables, is obtained by measuring: biomass, glucose, dissolved ethanol, oxygen and carbon dioxide.

A computer and other hardware are linked to the system in order to implement data acquisition, monitoring and open and closed control loop strategies (in open loop to impose constant or variable feed flow and in closed loop to test PID laws and adaptive control algorithms).

Micro system

The mini-system under development [4] for production of baker's yeast involves several modules: the bioreactor, the reading of the values of the variables to control (sensors), the data acquisition and signal conditioning systems, the control module for each system variable and the module for the actuators.

The mini-system for baker's yeast production is represented in the Figure 2. In the illustration are defined the variables to control (pH, ethanol concentration, glucose concentration, biomass, oxygen concentration and the temperature). The data acquisition system is responsible for the reception of the signals obtained through the reading of the sensors. It is linked to a computer that will allow monitoring and control.

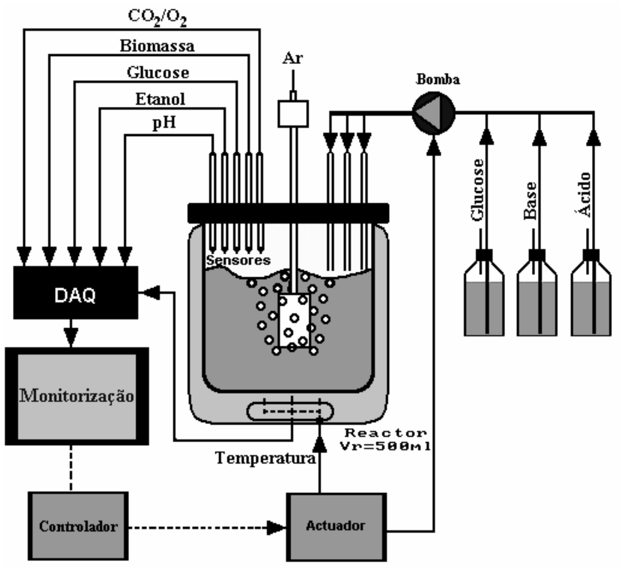

FIGURE. 2
MINI SYSTEM FOR BAKER'S YEAST FERMENTATION

Model equations

The conventional approach for fermentation process modeling is based on mass, energy and/or population balance equations. This form of modeling requires knowledge about reaction kinetics, thermodynamic, transport and physical properties.

The kinetic model for baker's yeast growth used in this work is based on the model presented by Sonnleitner and Käppeli [5], described and explained in [3]. Table I resumes mathematically the kinetic model knowing that only two of the three metabolic pathways coexist.

TABLE I
BAKER'S YEAST KINETIC EQUATIONS FOR THE RESPIRATIVE AND RESPIRO-FERMENTATIVE REGIMES

$aq_S \leq q_O$ Respirative Regime		$aq_S > q_O$ Respiro-Fermentative Regime	
$\mu_S^O = Y_{X/S}^O . q_S$	(1.a)	$\mu_S^O = Y_{X/S}^O \cdot \frac{q_O}{a}$	(2.a)
$\mu_S^r = 0$	(1.b)	$\mu_S^r = Y_{X/S}^r \cdot \left(q_S - \frac{q_O}{a} \right)$	(2.b)
$\mu_E^O = min\left(\mu_{E_1}^O , \mu_{E_2}^O \right)$	(1.c)	$\mu_E^O = 0$	(2.c)
$\mu_{E_1}^O = \mu_E^{max} \frac{E}{E + K_E} \frac{K_i}{S + K_i}$	(1.d)		
$\mu_{E_2}^0 = \frac{Y_{X/O}^{OE}}{Y_{X/E}^{OE}} \left(q_O - aq_S \right)$	(1.e)		

where S represents glucose; O oxygen; X biomass; E ethanol; C carbon dioxide, μ_S^o, μ_S^r, μ_E^o the specific growth rates for the three pathways, $Y_{X/S}^O$ and $Y_{X/S}^r$ represent the yield coefficients of biomass in glucose in the oxidative and fermentative phases, respectively, $Y_{X/E}^{OE}$ is the yield coefficient of biomass in ethanol in the oxidative phase in ethanol, $\mu_E^{\max}$ is the maximal specific growth rate, K_i is the inhibition parameter, K_E is the saturation parameter, q_S and q_O the glucose and oxygen uptake.

The mechanistic model for the fed-batch fermentation is obtained from mass balances for all the components considering that the reactor is well mixed [3]. Considering that the yield coefficient, *Y*'s, are constant and the dynamics of the gas phase can be neglected, the following set of differential equations was obtained:

- Mass balance for the biomass

$$\frac{dX}{dt} = -DX + \left(\mu_s^o + \mu_r^s + \mu_E^o\right) X \tag{3}$$

- Mass balance for the sugar

$$\frac{dS}{dt} = \left(-\frac{\mu_s^o}{Y_{x/s}^o} - \frac{\mu_s^r}{\mu_{x/s}^r}\right) X + \left(S_f - S\right) D \tag{4}$$

where S_f is the substrate concentration in the feed and D the dilution rate (feed rate/volume).

- Mass balance for the ethanol

$$\frac{dE}{dt} = \left(\frac{\mu_s^r}{Y_{X/E}^r} - \frac{\mu_E^O}{Y_{X/E}^{OE}}\right) X - DE \tag{5}$$

- Mass balance for the oxygen

$$\frac{dO}{dt} = \left(-\frac{\mu_s^O}{Y_{X/O}^O} - \frac{\mu_E^O}{Y_{X/O}^{OE}}\right) X - DO + OTR \tag{6}$$

- Mass balance for the carbon dioxide

$$\frac{dC}{dt} = \left(\frac{\mu_s^O}{Y_{X/C}^O} + \frac{\mu_s^r}{Y_{X/C}^r} + \frac{\mu_E^O}{Y_{X/C}^{OE}}\right) X - DC - CTR \tag{7}$$

- Accumulation of the working volume during the fed-batch process

$$\frac{dV}{dt} = F = DV \tag{8}$$

The gas transfer rates are given by:

$$OTR = K_L^O a\left(O^* - O\right) \quad \text{and} \quad CTR = K_L^C a\left(C - C^*\right) \tag{9}$$

where $K_L^i a$ are overall mass transfer coefficients for oxygen and carbon dioxide and O^* and C^* are the corresponding equilibrium concentrations.

Productivity and global efficiency equations

In the fed-batch fermentation the productivity can be estimated as the amount of biomass produced by unit of time and by unit of added volume represented by the following expression:

$$\text{Prod} = \frac{X_f V_f - X_0 V_0}{\left(V_f - V_0\right) t_f} \tag{10}$$

where the subscripts 0 and f refer to the initial and final conditions of the fermentation process.

The global efficiency of biomass relatively to the substrate is calculated as:

$$\text{Rend} = \frac{X_f V_f - X_0 V_0}{\int_0^{t_f} F S_E\, dt + S_0 V_0 - S_f V_f} \tag{11}$$

BAKSIM DEVELOPMENT

This application was developed using the platform LabVIEW and the data acquisition board 6024E, both from National Instruments.

BakSIM can operate in one of three operation modes: simulation, monitoring and monitoring with simulation.

Simulation

The simulation mode uses the kinetic equations (1-2) and the mass balance equations (3-9) and, with appropriate integration methods, predicts the behavior of the concentration of the state variables over a 20 hours time period, in a well-mixed reactor. The kinetic [5] and yield coefficients [6] parameters considered in the model can be obtained from the literature.

The simulation mode can operate in two modes: open loop mode and close loop mode.

In open loop mode there is no control of the ethanol concentration level, in opposition with closed loop mode where the control is possible through a PID algorithm that operate on the feed flow substrate.

This routine makes possible to the user to define the initial parameters and conditions for the respective simulation, Figure 3. The user can modify the kinetics parameters and yield coefficients that were considered [3].

As the simulation runs, the user can observe the concentration profiles of all six state variables (Figure 4).

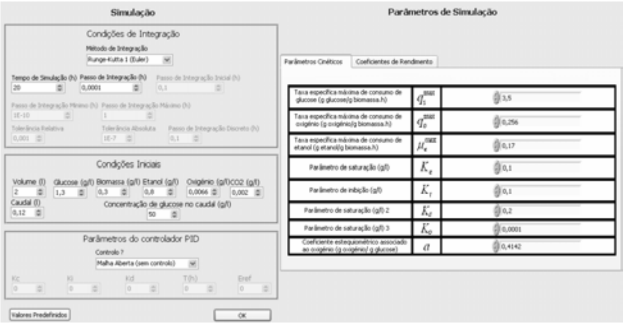

FIGURE 3
SIMULATION DATA INTRODUCTION

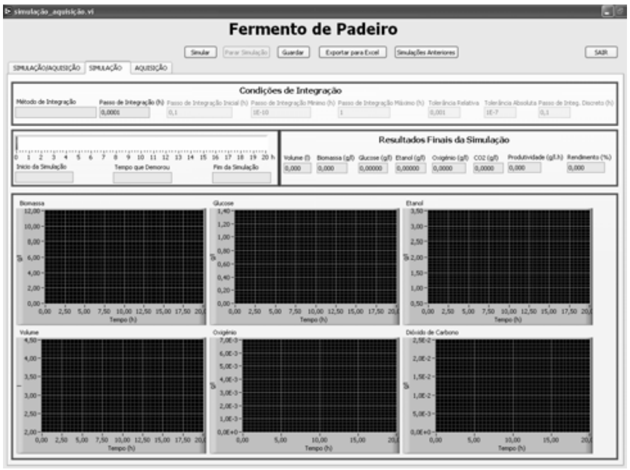

FIGURE 4
SIMULATION INTERFACE

Monitoring

The monitoring operation mode is used to process and to analyze the signals generated from the experience acquired by the data acquisition board, Figure 5.

Simulation/Monitoring

The simulation/monitoring operation mode executes the two previous modes simultaneously. The Figure 6 shows de interface developed for this operation mode.

Others functions

In addition to the three operation modes previously described, this application makes possible other functionalities: to read and to keep the most important parameters of a simulation or acquisition in an ACCESS data base. All the results concerning to a particular simulation process or acquisition can be read and used by EXCEL for others analyses.

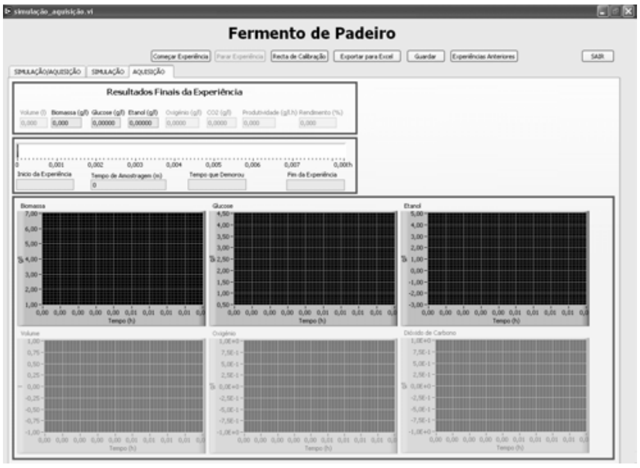

FIGURE 5
MONITORING INTERFACE

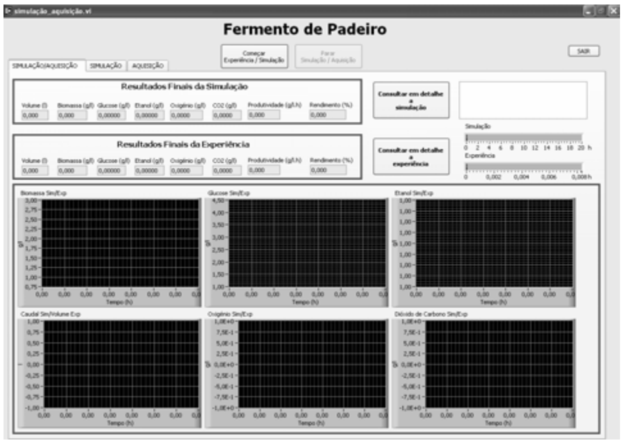

FIGURE 6
SIMULATION/MONITORING INTERFACE

RESULTS

The BakSim application developed was then used to simulate the baker's yeast growth process. Two examples will be presented: one for the open loop mode and other for the close loop mode.

Open loop mode

To test the operation of BakSIM application in open loop mode, we run a simulation of 20h of operation time with an initial volume of 2.5l. The initial value of the concentration of glucose in the feed was 50 g/l and a feed flow constant at 0.12l. The initial conditions for the state variables are in the Table II.

The application allows the use of several numeric methods to carry out the simulation. Several simulations were carried out in order to verify the adequate numerical methods to simulate the fermentation process. The Runge-

Kutta 4 was chosen due to its efficiency. In Figure 7 are the concentration profiles for the state variables and in Table III the correspondent's final concentration vales.

TABLE II
INITIAL CONDITIONS FOR THE STATE VARIABLES

X (g/l)	*S* (g/l)	*E* (g/l)	*O* (g/l)	CO_2 (g/l)
1.20	1.46	2.27	0.0066	0.002

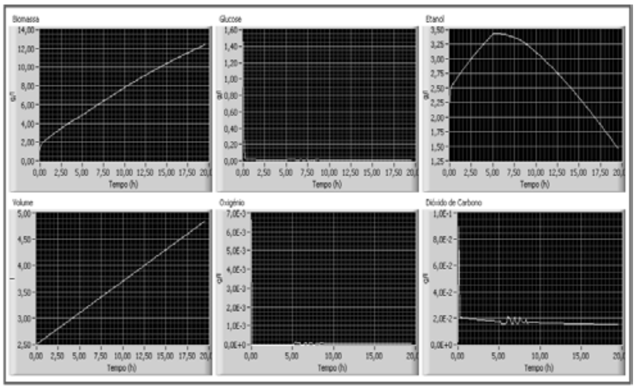

FIGURE 7
SIMULATION FINAL CONCENTRATION PROFILES FOR THE STATE VARIABLES

TABLE III
SIMULATION FINAL CONCENTRATION VALUES FOR THE STATE VARIABLES

X	*S*	*E*	*O*	CO_2	*V*	Prod.	Rend.
(g/l)	(g/l)	(g/l)	(g/l)	(g/l)	(l)	(g/l.h)	(%)
12.39	0.005	1.467	$2.6e^{-5}$	0.015	4.84	1.249	47.25

Close loop mode

This operation cannot be tested with real parameters, given that the measurement systems of the respective concentrations are still under development.

CONCLUSIONS

This work describes an experience based on the final project work for the Industrial Electronics Engineering undergraduate course. An application for the simulation and monitoring of the baker's yeast fermentation was developed in the platform LabVIEW. Besides the main goal defined for this work, some extra functionalities were implemented, such as: to allow to export the resulting data of the simulations or experiences to EXCEL, as well to keep the same ones in the data base ACCESS, facilitating the creation of reports.

The developed numeric methods routine for the simulation makes available a group of numeric methods for the resolution of the set of differential equation that defines the baker's yeast fermentation mathematical model. It also permits the comparison of the effectiveness of the numerical methods on the simulation.

The BakSim application revealed quite useful in this type of experiences since reduces the time face to a real experience of baker's yeast production that it takes up to 15 a 20 hours, allowing to test different parameters in a short interval of time.

To finalize must be point out that this project was relevant for its multidisciplinary work since incorporates several areas as Programming, Process Control and Numerical Methods.

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