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COMPUTER MODEL FOR THE GROWTH BEFORE SPORULATION OF A FUNGAL POPULATION ON SOLID SUBSTRATE

R. ALONSO F. (*), M. RODRÍGUEZ R. (*), I. LÓPEZ S. (*) and G. GUERRA R. (**)
(*) Fac. of Mathematics, (**) Fac. of Biology, Havana University, Cuba

Abstract

We show numerical results of a system conformed by two ordinary differential equations coupled with a diffusion equation, arising in a previous model of differentiated growth of fungal biomass governed by the oxygen present at different levels. Using finite differences we solve the diffusion problem and compare the influence of different boundary conditions. Times of biomass changes from vegetative to competent at each depth-level inside the medium are determined. Calculations of the critical substrate thickness and the distribution of biomass respect to time and depth, are showed. The oxygen flow through the open boundary is also studied.

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1. Introduction

It's well known the importance of solid substrate fermentation process [1]. This paper is devoted to the numerical treatment and results of a model of a fungal population on solid substrate based in [2], which consists in a system of equations representing respectively the evolution of differentiated fungal biomass and the oxygen diffusion.

We consider the biomass distributions and oxygen concentration depending in only one spatial coordinate (relative depth) and, on time. Here all parameters and unknowns are dimensionless, starting from appropriate scales. There are two consequences of this model:
(a) the mathematical evidence of a delay (which increases monotonously as depth increases) in the biomass evolution inside a substrate which fill a reactor (box without lid) and;
(b) the existence of a critical thickness (CT) of the substrate column representing the maximal thickness for which all the biomass inside the reactor is competent at the moment of sporulation on the upper boundary (UB). These mathematical facts are in agreement with the experimental evidence.

The paper is divided as follows. Section 2 is devoted to the formulation of the model. In Section 3 is resumed the numerical scheme. We present, in Section 4, the way of dependence on depth of time-values in which a phase change occurs inside the medium and further, the way in which biomass depend on time and depth. We reserve Section 5 to the procedure and calculation of CT and critical values (J^2_{crit}) of the nondimensional parameter J^2 involving physical and biological characteristics of the process. We show the connection between J^2_{crit} and CT. In Section 6 we include the analysis of the flow parameters representing the initial gradient and the diffusion celerity at the superior open surface, through numerical calculations. Conclusions are given in Section 7. References were included in Section 8. Finally, we present some graphics showing general aspects of the studied dependencies.

2. Formulation of the Model

The system representing the kinetics of differentiated biomass formation at the ζ-depth is given by two equations, which are, in 4each

depth inside the reactor, respectively valid for lesser or greater time-values than the time of change $t^*(\zeta)$. Let us denote by $X_i(\zeta,\tau)$ the distribution (see [4] Chap.4 for other quantification of the biomass) of differentiated biomass: vegetative ($i=1$); competent ($i=2$). We refer to [2] for more details. A Monod law is assumed, provided $\tau < t^*(\zeta)$:

$$\frac{dX_1}{d\tau} = m\Gamma(\zeta,\tau)\,X_1 \tag{2.1}$$

and, if $\tau > t^*(\zeta)$, is present a generalization of Monod law like in [2] :

$$\frac{dX_2}{d\tau} = [m\Gamma(\zeta,\tau) - n_1 - n_2]\,X_2 \tag{2.2}$$

where $\Gamma(\zeta,\tau) = \frac{\Omega_0}{\Omega_0+\frac{1}{\varepsilon}}$.

The equation for the oxygen density taking into account diffusion and consumption is:

$$\frac{\partial\Omega_0}{\partial\tau} = d\cdot\frac{\partial^2\Omega_0}{\partial\zeta^2} - \left(eX^0\right)\Omega_0 \tag{2.3}$$

The above system describes main approximations of biomasses (X_i) an oxygen concentration (Ω_0), and was obtained in [2] uncoupling a more complex system by a perturbation expansion in powers of , the inverse of the affinity constant of oxygen. There, was obtained the approximate value of d provided ε small :

$$d \approx J^2 = \frac{DT^*}{H^2C} \tag{2.4}$$

where $C = V_T^{-1}\left(V_P - \frac{\alpha}{\rho}\int_0^1 X^0(\zeta)\,d\zeta\right)$ be a constant involving the relative pore volume at the initial moment. Previously, the spores were homogeneously distributed in the medium.

The initial conditions for the system at each level are given by:

$$\begin{array}{c} X_1(\zeta,0) = X_1^0(\zeta) \\ X_2(\zeta,t^*(\zeta)) = X_1(\zeta,t^*(\zeta)) \end{array} \tag{2.5}$$

$$\Omega_0(\zeta,0) = \Omega_*(\zeta) \tag{2.6}$$

In [2] were considered the boundary conditions on the UB and bottom:

$$\Omega_0(0,\tau) = 1 \tag{2.7}$$

$$\frac{\partial \Omega_0}{\partial \zeta}(1,\tau) = 0. \tag{2.8}$$

Further, we consider here the following boundary condition instead of (2.7):

$$\frac{\partial \Omega_0}{\partial \zeta}(0,\tau) = f \cdot \exp(-p\tau) \tag{2.9}$$

where the physical meaning of parameters f and p are indicated in Section 6.

3. The Numerical Scheme

Our first problem is to solve (3) with the initial and boundary conditions for the oxygen concentration, discretized by finite differences. This procedure leads to a symmetric implicit Crank-Nickolson scheme, which is solved by the factorization method. We estimate the deviation order by standard methods, and prove the stability of both schemes respect to the right member. Further, all equations in the scheme representing the diffusion equation and the initial and boundary conditions appears with the required approximation in order to guarantee the convergence of schemes. In [5] was presented a detailed description of the numerical scheme alluded here.

Finally we use the obtained values of the oxygen concentration for the integration of the biomass equation (Eq. 2.1) at each ζ-level inside the medium.

4. Calculation for $t^*(\zeta)$.

In [2] were derived formulas for time-values $t^*(\zeta)$, which are the times needed at depth ζ to obtain quantities of differentiated biomasses equal to those present on the UB at the instant $t^*(0)$.

In [2] was obtained the following implicit formula:

$$\int_0^{t\cdot *(\zeta)} \Omega_0\left(\zeta, t\right) dt = \int_0^{t^*(0)} \Omega_0\left(0, t\right) dt. \tag{4.1}$$

To calculate these time-values for biomass phase changes we use Newton's method. In the approximation of the integrals we use the rule of trapezia, for which the values $\Omega_0\left(\zeta, t^i\left(\zeta\right)\right)$ were determined by linear interpolation provided $t_j < t^i\left(\zeta\right) < t_{j+1}$.

5. Critical Value of J^2.

For practical uses an important question follows, How can we estimate the CT of the medium? Hence, we introduce the critical value J^2_{crit} as the value of this parameter for which $t^*\left(1\right) = 1$. We may rewrite (4.1) as,

$$\int_0^1 \Omega_0\left(1, t;^2\right) dt = \int_0^{t^*(0)} \Omega_0\left(0, t; J^2\right) dt. \tag{5.1}$$

The value J^2_{crit} satisfying (5.1) strongly depends on (eX^0), $t^*\left(0\right)$, and weakly on Ω_*. Further, it depends also on f and p provided condition (2.9). The values J^2_{crit} and CT, are connected by (2.4).

To determine J^2_{crit} for a selected set of parameters we use the secant method. If we denote by $(J^2_s)_{s\in N}$ the convergent sequence to J^2_{crit}, we calculate the integrals

$$\int_0^{t^*(\zeta)} \Omega_0\left(\zeta, t : J^2_s\right) dt$$

$\zeta \in \{0, 1\}$, by the rule of trapeze. Using the Linear Interpolation Method in determining each new value in the sequence, and fixing $\Omega_* = \exp\left(-2\xi\right)$, $t^*\left(0\right) = 0.3$, $(eX^0) = 0.04$, we obtain

$$J^2_{crit} = 147.638331559$$

for the boundary condition (2.9) when $f = -1.79245$ and $p = 140$.

6. Flow Parameters at the upper Boundary

Flow parameters f, p at the UB were presented in (2.9), representing the initial value of the gradient and the flow celerity at this surface. These parameters are coupled in a closely way with the parameter J^2. Hence, if the intention of the model requires the boundary condition (2.9), then we need to clarify all connections between them. To do so, the procedure is based on the fact that limit values of the oxygen concentration at the UB as time goes to infinity should be the same as the corresponding value outside the medium. This is a natural condition, but in reality our equations do not model completely the evolution of the biomass for long times. Nevertheless, it serves at least for an asymptotic estimate near the oxygen equilibrium.

This procedure allows us to solve numerically the implicit equation:

$$\lim_{t\longrightarrow\infty} \Omega_0\left(0, t; J^2; f; p\right) = 1 \tag{6.1}$$

and, we select a value of any of the three parameters in the equation and show the dependence between the others using a numerical procedure similar to those used to obtain neutral stability curves in Hydrodynamics. The results of the corresponding transcendental equations are showed in Figs.1,2,3, in which the value of the fixed parameter in each case was selected from the set:
$\{J^2 = 147.638332,\, p = 140,\, f = -1.79245\}$.

7. Discussion

In this paper we numerically show the influence of different non-dimensional parameters representing physical and biological characteristics on the biomass in a solid substrate fermentation reactor. We mainly focused our attention on the determination of the parameter J^2_{crit}. From (2.4) we estimate the CT.

In Fig.4 we show time dependencies of oxygen concentrations at different depths inside the reactor, provided condition (6.3). A very similar portrait can be also obtained for condition (6.1), as can be seen in [2]. In Fig.5 is shown how depends on time the total amount of biomass at different depths inside, for selected values of parameters.

It is shown in Fig.6 the dependence of phase change times at different depths inside the reactor for values of near to the critical. Considering (2.7), in Figs.7,8 we show partial dependencies of J^2_{crit} with respect to (eX_0) and $t^*(0)$. These graphics obtained from the numerical calculations, very much agree with the analytically computed in [2]. A more detailed biological discussion complemented with experimental data was presented in [6].

8. References

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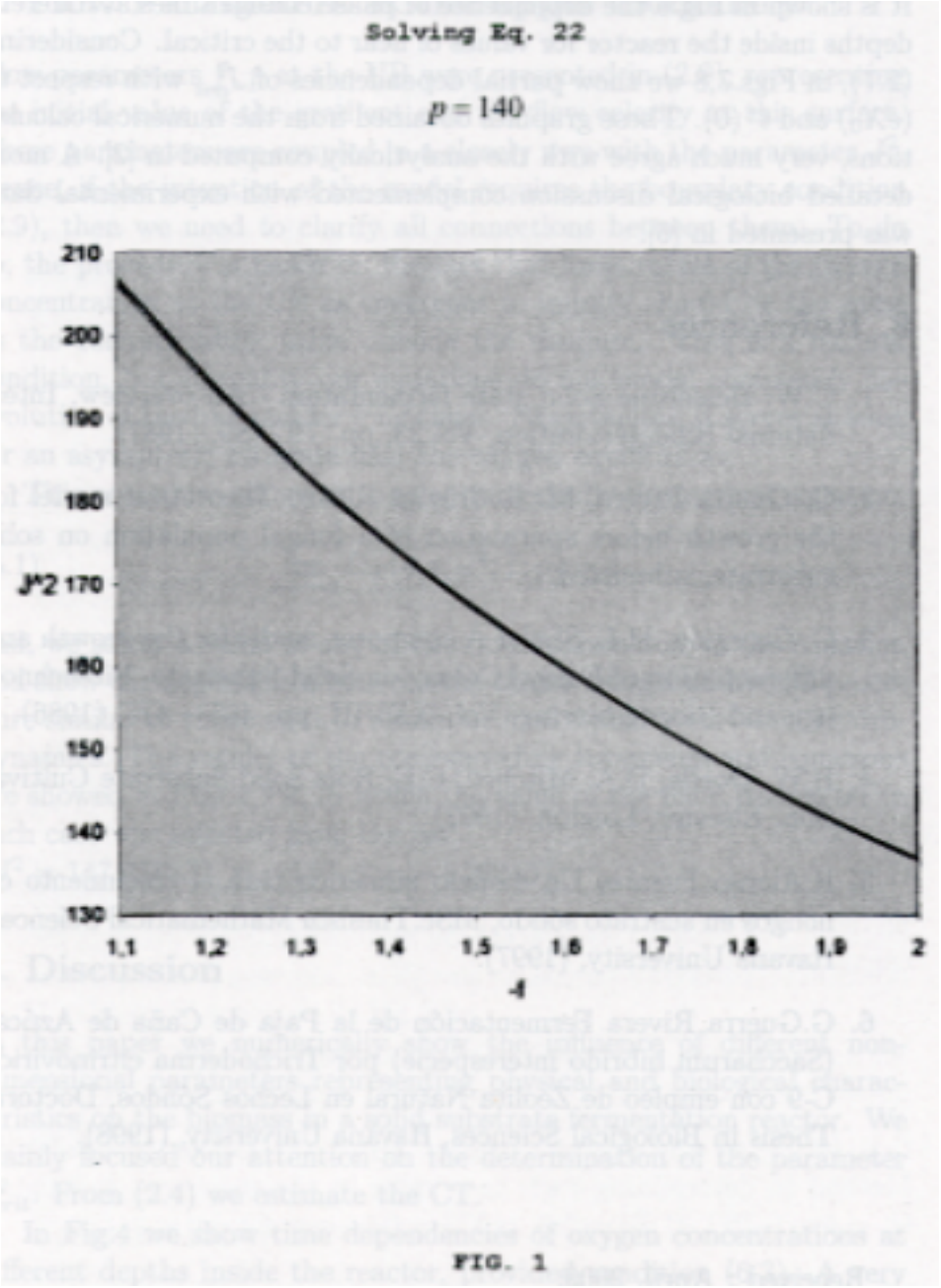

Solving Eq. 22
p = 140
210
200
190
180
J^2 170
160
150
140
130
1,1
1,2
1,3
1,4
1,5
1,6
1,7
1,8
1,9
2
-f

FIG. 1

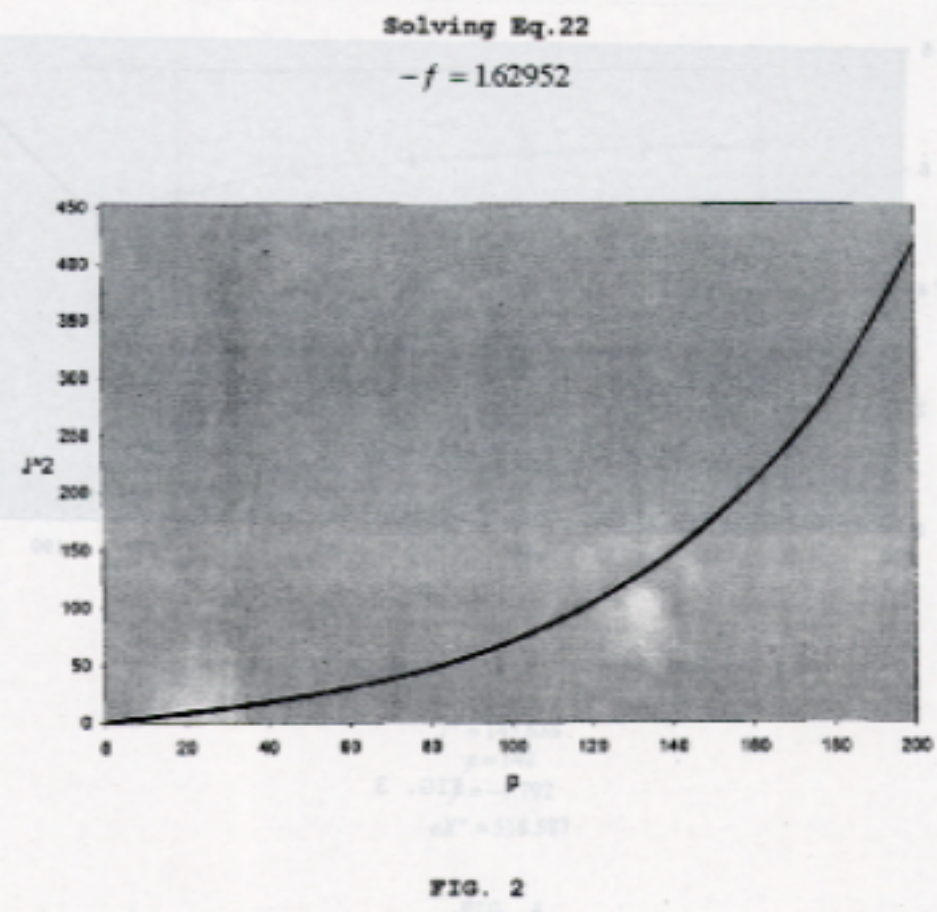

Solving Eq.22
$-f = 162952$
450
400
350
300
250
J^2
200
150
100
50
0
0
20
40
60
80
100
120
140
160
180
200
p

FIG. 2

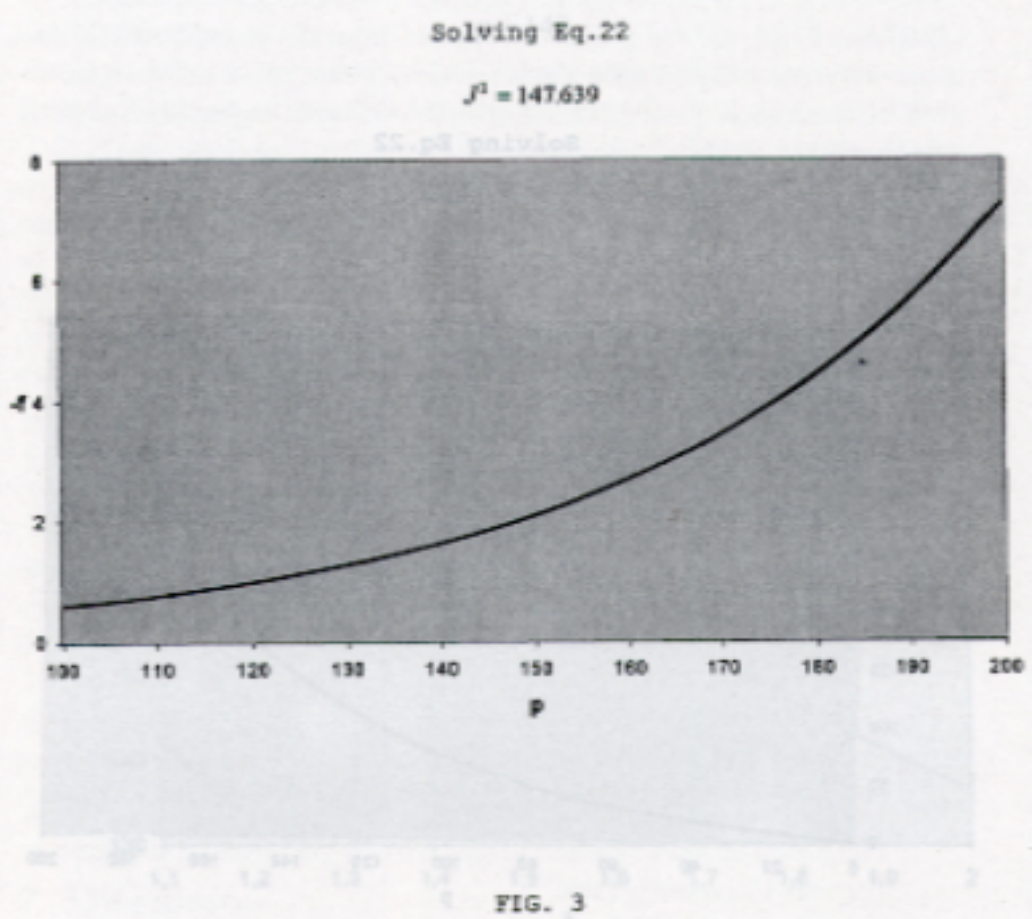
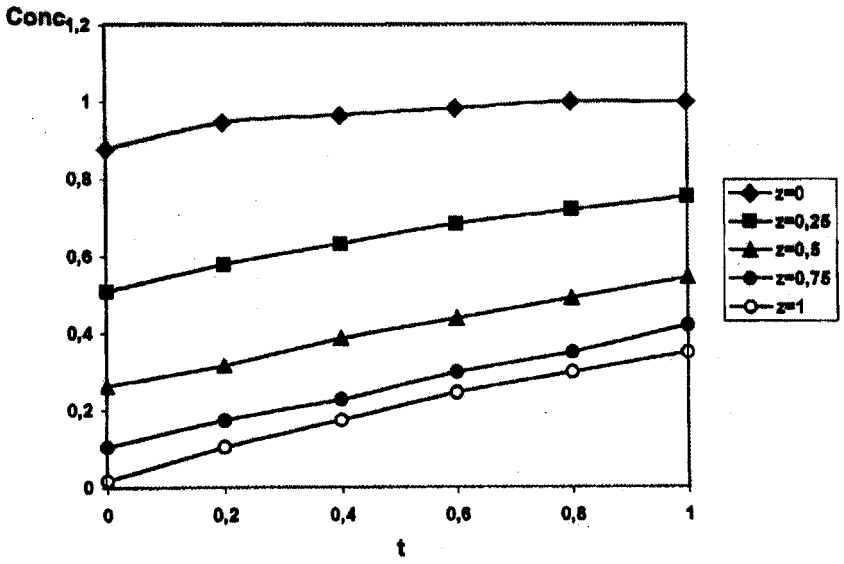

Solving Eq.22
$J^1 = 147.639$
8
6
4
2
0
100
110
120
130
140
150
160
170
180
190
200
P

FIG. 3

Oxygen Concentration

Condition (6.3)



Initial biomass distribution: $\exp(-2z)$

$J^2 = 147.638$
$p = 140$
$f = -1.792$
$eX^o = 518.587$

FIG. 4

R. Alonso Fuentes
M. Rodríguez Ricard
I. López Saura
Facultad de Matematicas y Computación
Universidad de la Habana
Ciudad de la Habana 10400
Cuba

and

G. Guerra Rivera
Facultad de Biología
Universidad de la Habana
Ciudad de la Habana 10400
Cuba