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Solutions of Balance-Transport Models for (Solid-State Fermentation) Bioreactors with Infinite Diffusion

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Abstract The models used to examine the processes of the solid-state fermentation bioreactors can be improved using the heat and mass transfer models compared to empirical models. This study examines the oxygen balance equations, water balance and energy balance equations for solid-state fermentation bioreactors. For the precise study of these important transport problems some advanced ingredients of applied mathematics such as sobolev spaces, weak solutions, Galerkin method, Gronwall's inequality and Harnack's inequality has been used. Based upon these concepts, the solutions of the balance equations for bioreactors is presented. By the proposed method, the uniqueness of the solutions of the balance equations has been proved. This procedure leads to a general methodology for reducing these initial/boundary partial differential equations to a system of ordinary differential equations which easily can be solved. It is also shown in this structure that the solution is the best answer since it supports the infinite diffusion speed of disturbances.

Keywords: *heat and mass transfer model, solid state fermentation bioreactor, balance-transport models, parabolic boundary value problem, weak solution*

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1. Introduction

Transport phenomena, especially heat transfer and mass transfer are significant issues in the study of various biology and chemistry problems. Especially, in biology, some of the kinetic models used to describe the growth kinetics of solid fermentation (SSF) can predict many important parameters such as specific growth rates, process performance, process efficiency, generated heat, process control measures, strategy for the production of specific products and industrial scale considerations.

Models that consider both temperature and moisture in examining the effect of environmental conditions on microbial growth can be used in studies on heat transfer and mass transfer in SSF processes.

In general, it can be assumed that stoichiometric models with a focus on microbial pathways can predict the behavior of microorganisms and can be suitable for simple experimental models in SSF processes. These models can be improved with heat and mass transfer models compared to empirical models, and further studies on SSF are needed in this regard. For this purpose, mathematical modelling based on heat transfer and mass transfer problems can be used to investigate such problems, [1-5].

On the other hand, despite the greater interest in the production of microbial products by solid-state fermentation (SSF), using this large-scale culturing method, due to the relatively poor heat and mass transfer in the solid particle bed, there are great challenges against it in the SSF bioreactors.

Mathematical models and computational simulations are useful tools to make operational and control strategies to overcome these challenges and can be applied to the simulation of oxygen consumption, heat production and cell growth in a fermentation state (SSF).

Not only do these models direct the design and function of the bioreactors, but they can also combine their insights on how different phenomena within the fermentation system control the overall process performance. Also, the extent of the limitation will be analyzed due to the phenomenon of heat transfer and/or mass at different stages of fermentation, ([6-12]).

As mentioned above, various mathematical modelling has been performed to optimize the design and operation of solid-state fermentation bioreactors (SSF). These models are designed to partially describe the transport phenomena in the bed and the exchange of mass and energy between the bed and the bioreactor subsystems, such as the bioreactor wall and headspace gases.

What is being discussed in this paper is the study of the existence and uniqueness of the answer to the models of various transport phenomena. The method chosen for solving is one that is superior to numerical and approximate methods such as Galerkin's method and others in terms of mathematical technique and in line with the insights obtained through modelling.

The proposed method can be used as a more powerful tool in optimizing the performance of the bioreactor and it also can be applied to the other complex nonlinear problems, [13-16].

After the statement of the problem in Section 2, the main result expressed and proved in Section 3. Also, the proposed methodology that is proving the existence and uniqueness of the weak solution of the general problem results in the reduction of the general initial/boundary PDE to a system of an ODE which easily can be solved.

The other advantage of the new approach is that the maximum of the function in some interior of the bioreactor at a positive time can be estimated by the minimum of it in the same region at a later time. This fact supports the infinite diffusion speed of disturbances. Then can be suitable for heat and mass–transfer models in (semi-infinite) SSF bioreactors with more diffusion.

2. Statement of the Problem

The balance-transport models listed in Table 1. These models describe mass and heat transfer in different phases of the bioreactor in order to predict how the flow rate, humidity and inlet air temperature affect the temperature and water content of the substrate.

Table 1. Description of balance-transport models

Equation	Description
$\frac{\partial C_{O_2}^b}{\partial t} = D_{O_2}^b \frac{\partial C_{O_2}^b}{\partial z^2} - r_{O_2}$ ([2]) $\frac{\partial C_\varepsilon}{\partial t} = D_{O_2}^b \frac{\partial^2 C_{O_2}}{\partial z^2} - K_a a_x \left(C_{O_2} - HC_{O_2}^f \right)$ ([9])	Oxygen balances for tray bioreactors (Indicates the conditions for O_2 diffusion within pores and uptake by microorganisms.)
$\frac{\partial C_W}{\partial t} = r_{H_2O} - \left[\frac{\partial C_{VAP}}{\partial t} - D_{VAP}^* \frac{\partial^2 C_{VAP}}{\partial z^2} \right]$ ([2])	Water balances for tray bioreactors (Describes the water balance in the substrate bed within the tray)
$\rho_s C_{sp} \frac{\partial T}{\partial t} = k_b \frac{\partial^2 T}{\partial z^2} + r_Q$ ([9,10]) $\frac{\partial H}{\partial t} = K_b \frac{\partial^2 T}{\partial z^2} + r_Q + \lambda D_{VAP}^* \frac{\partial^2 C_{VAP}}{\partial z^2}$ ([2])	Energy balances for tray bioreactors (Takes into account conduction and metabolic heat production)

Table 2. Description of the parameters of Table 1

Parameters	Description
t	time
$C_{O_2}^b$	concentration of O_2 per unit volume of the bed
z	vertical coordinate
r_{O_2}	rate of O_2
$D_{O_2}^b$	diffusion of O_2
ε	porosity of the bed
K_a	mass transfer coefficient for O_2 at the air/biofilm interface
a_x	area of the air/biofilm interface per unit volume of the bioreactor
H	Henry's law constant
$C_{O_2}^f$	concentration of O_2 within the biofilm
C_W	liquid water concentration per unit volume of bed
C_{VAP}	water vapor concentration per unit volume of bed
D_{VAP}^*	effective diffusion coefficient of water vapor within the bed
r_{H_2O}	metabolic rate of water production
ρ_s	density of the bed
C_{sp}	heat capacity of the bed
T	bed temperature
K_b	thermal conductivity of the bed
r_Q	rate of metabolic heat production by the microorganism

3. Solution of the Balance Equations for Bioreactors

Theorem. The (weak) solution of oxygen balance equations, water balance and energy balance equations for bioreactors exists and is unique. Also, the obtained solution supports infinite diffusion speed of disturbances. Then can be suitable for heat and mass–transfer models in (semi-infinite) SSF bioreactors with more diffusion.

Proof. Consider an open, bounded subset U of $\mathbf{R}^n$. Consider the initial/boundary-value such as

$$\begin{cases} u_t + Pu = f, & in\ U_T \\ u = 0, & on\ \partial U \times [0,T], \\ u = g, & on\ \partial U \times \{t=0\}, \end{cases} \quad (1)$$

Where $U_T = U \times (0,T]$ for some fixed time $T > 0$, $f : U_T \to \mathbf{R}$ and $g : U \to \mathbf{R}$ are given, and $u : \overline{U_T} \to \mathbf{R}$ is the unknown; $u = u(x,t)$. The letter P denotes a second–order partial differential operator for each time t with the nondivergence form

$$Pu = -\sum_{i,j}^{n} a^{ij}(x,t) u_{x_i x_j} + \sum_{i=1}^{n} b^i(x,t) u_{x_i} + c(x,t)u \quad (2)$$

for given coefficients $a^{ij}, b^i, c \quad (i,j = 1,\ldots,n)$.

Let $a^{ij}, b^i, c \in L^\infty(U_T)$, $f, g \in L^2(U_T)$ and $a^{ij} = a^{ji}$ $(i,j = 1,\ldots,n)$. The time–dependent bilinear form has been defined as

$$f[u,v;t] = \int_U \sum_{i,j}^{n} a^{ij}(.,t) u_{x_i} v_{x_j} + \sum_{i=1}^{n} b^i(.,t) u_{x_i} v + c(.,t) u dv \quad (3)$$

For $u, v \in H_0^1(U)$, $0 \le t \le T$ almost everywhere.

Let $u(x,t)$ is a smooth solution of the parabolic problem (1). To change the point of view, associate with u a mapping, $u : [0,T] \to H_0^1(U)$ defined by

$$[u(t)](x) := u(x,t) (x \in U, 0 \le t \le T)$$

Returning to problem (1), similarly define $f : [0,T] \to L^2(U)$ such that

$$[f(t)](x) := f(x,t), (x \in U, 0 \le t \le T)$$

Fixing a function $v \in H_0^1(U)$ and integrating by parts lead to

$$(\mathbf{u}', v) + F[\mathbf{u}, v; t] = (\mathbf{f}, v), \left(' = \frac{d}{dt} \right), \quad (4)$$

for each $0 \le t \le T$, the pairing $(,)$ in equation (4) denoting inner product in $L^2(U)$ and F is defined as the equation (3). Then

$$u_t = g^0 - \sum_{j=1}^{n} g_{x_j}^j, \quad in\ U_T \quad (5)$$

For

$$g^0 = f - \sum_{i=1}^{n} b_i u_{x_i} - cu$$

and

$$g^j = \sum_{i=1}^{n} a^{ij} u_{x_i} - cu \ (i,j = 1,\ldots,n).$$

Thus the right hand side of (5) lies $H^{-1}(U)$. This estimate suggests it may be reasonable to look for a weak solution with $\mathbf{u}' \in H^{-1}(U)$ for almost everywhere time $0 \le t \le T$.

Then, reformulate the equations of Table 1 as Table 3:

Table 3. Description of balance-transport models

Balance Equation	Substitution	Heat Equation
$\frac{\partial C_{O_2}^b}{\partial t} = D_{O_2}^b \frac{\partial C_{O_2}^b}{\partial z^2} - r_{O_2}$	$C_{O_2}^b = u$	
$\frac{\partial C_\varepsilon}{\partial t} = D_{O_2}^b \frac{\partial^2 C_{O_2}}{\partial z^2}$ $-K_a a_x \left(C_{O_2} - HC_{O_2}^f \right)$	$C_\varepsilon - C_{O_2} = u$	
$\frac{\partial C_W}{\partial t} = r_{H_2O}$ $-\left[\frac{\partial C_{VAP}}{\partial t} - D_{VAP}^* \frac{\partial^2 C_{VAP}}{\partial z^2} \right]$	$C_W - C_{VAP} = u$	$u_t + Pu = f$
$\rho_s C_{sp} \frac{\partial T}{\partial t} = k_b \frac{\partial^2 T}{\partial z^2} + r_Q$	$T = u$	
$\frac{\partial H}{\partial t} = K_b \frac{\partial^2 T}{\partial z^2}$ $+r_Q + \lambda D_{VAP}^* \frac{\partial^2 C_{VAP}}{\partial z^2}$	$-T = u$	

The initial/boundary value problem (1) covers all of the models which expressed in Table 3 and they can be reformulated to the form of (2). Therefore, the only remaining work is to examine the existence and uniqueness of their answer.

Assume the functions

$$\varphi_k = \varphi_k(x)(k = 1,\ldots,m)$$

are smooth, and $\{\varphi_k\}_{k=1}^\infty$ is an orthogonal basis of $H_0^1(U)$ and is an orthonormal basis of $L^2(U)$. Fix a positive integer *m.* In this way, a function $\mathbf{u}_m : [0,T] \to H_0^1(U)$ of the form

$$\mathbf{u}_m(t) := \sum_{k=1}^{m} \rho_m^k(t) \varphi_k \quad (6)$$

can be found with the coefficients

$$\rho_m^k(t)(0 \le t \le T, k = 1,\ldots,m)$$

of the form

$$\rho_m^k(0) = (g, \varphi_k), \quad (7)$$

for $(k=1,...,m)$ and satisfies the equation

$$\begin{aligned}&(\mathbf{u}'_m,\varphi_k)+F[\mathbf{u}_m,\varphi_k;t]=(\mathbf{f},\varphi_k)\\&(0\le t\le T,k=1,...,m)\end{aligned}\tag{8}$$

where, $(,)$ denotes the inner product in $L^2(U)$.

In this way, the problem converts to the Finding a function $\mathbf{u}_m$ of the form (6) which satisfies the projection (7) of problem (1) onto the finite dimensional subspace spanned by $\{\varphi_k\}_{k=1}^{\infty}$.

For this purpose, assume that $\mathbf{u}_m$ has the structure (6), then

$$(\mathbf{u}'_m,\varphi_k)=\rho_m'^k(t).$$

Furthermore, for $k,l=1,...,m$

$$F[\mathbf{u}_m,\varphi_k;t]=\sum_{l=1}^{m}e^{kl}(t)\rho_m^l(t),\ e^{kl}(t)=F[\varphi_l,\varphi_k;t].$$

Let

$$f^k(t):=(f(t),\varphi_k)(k=1,...,m),$$

then (8) becomes the linear system of ODE

$$\rho_m'^k(t)+\sum_{l=1}^{m}e^{kl}(t)\rho_m^l(t)=f^k(t),\ (k=1,...,m)\tag{9}$$

subject to the initial conditions (7). There exists a unique absolutely continuous function

$$\rho_m(t):=\left(\rho_m^1(t),...,\rho_m^m(t)\right)$$

satisfying (7) and (8) for almost everywhere $0\le t\le T$.

It will be shown a subsequence of the solutions $\mathbf{u}_m$ of approximate problems (8), (9) converges to a weak solution of (1). For this, some uniform estimates such as energy estimates will be necessary which states there exists a constant c, depending only on U,T and the coefficients of L, such that

$$\begin{aligned}&\max_{0\le t\le T}\|\mathbf{u}_m(t)\|_{L^2(U)}+\|\mathbf{u}_m(t)\|_{L^2(0,T;H_0^1(U))}\\&+\|\mathbf{u}'_m(t)\|_{L^2(0,T;H_0^1(U))}\\&\le c\left(\|\mathbf{f}\|_{L^2\left(0,T;L^2(U)\right)}+\|g\|_{L^2(U)}\right),\quad\forall m=1,2,\end{aligned}\tag{10}$$

According to the energy estimates (10), it can be seen that the sequence $\{\mathbf{u}_m\}_{m=1}^{\infty}$ is bounded in $L^2\left(0,T;H_0^1(U)\right)$, and $\{\mathbf{u}'_m\}_{m=1}^{\infty}$ is bounded in $L^2\left(0,T;H_0^{-1}(U)\right)$.

Consequently, there exists a subsequence $\{\mathbf{u}_{m_l}\}_{l=1}^{\infty}\subset\{\mathbf{u}_m\}_{m=1}^{\infty}$ and a function

$$\mathbf{u}\in L^2\left(0,T;H_0^1(U)\right)$$

with

$$\mathbf{u}'\in L^2\left(0,T;H_0^1(U)\right)$$

such that

$$\begin{cases}\mathbf{u}_{ml}\to\mathbf{u},\ \textit{weakly in } L^2\left(0,T;H_0^1(U)\right)\\ \mathbf{u}_{ml}\to\mathbf{u}',\ \textit{weakly in } L^2\left(0,T;H_0^{-1}(U)\right)\end{cases}\tag{11}$$

Next fix an integer N and choose a function $\mathbf{v}\in C^1\left([0,T];H_0^1(U)\right)$ having the form

$$\mathbf{v}(t)=\sum_{k=1}^{N}\rho^k(t)\varphi_k\tag{12}$$

where $\{\rho_k\}_{k=1}^{n}$ are given smooth functions. At this stage, respectively, choose $m\ge N$, multiply (8) by $e^k(t)$, sum on $k=1,...,N$, and then integrate with respect to t. This process results to

$$\int_0^T\langle\mathbf{u}_m,\mathbf{v}\rangle+F[\mathbf{u}_m,\mathbf{v};t]dt=\int_0^T(\mathbf{f},\mathbf{v})dt\tag{13}$$

Set $m=m_l$ and recall (11), to find upon passing to weak limits that

$$\int_0^T\langle\mathbf{u},\mathbf{v}\rangle+F[\mathbf{u},\mathbf{v};t]dt=\int_0^T(\mathbf{f},\mathbf{v})dt\tag{14}$$

This equality then holds for all functions $v\in L^2\left(0,T;H_0^1(U)\right)$, as functions of the form (12) are dense in this space. Hence in particular

$$\langle\mathbf{u},\mathbf{v}\rangle+F[\mathbf{u},\mathbf{v};t]=(\mathbf{f},\mathbf{v}),\ \forall v\in H_0^1(U),\tag{15}$$

furthermore, $\mathbf{u}\in C\left([0,T];L^2(U)\right)$. In order to prove $u(0)=g$, at first note from (14)

$$\begin{aligned}&\int_0^T-\langle\mathbf{v},\mathbf{u}\rangle+F[\mathbf{u},\mathbf{v};t]dt=\int_0^T(\mathbf{f},\mathbf{v})dt+(\mathbf{u}(0),\mathbf{v}(0))\\&\forall\mathbf{v}\in C^1\left([0,T];H_0^1(U)\right),\\&\mathbf{v}(T)\equiv 0\end{aligned}\tag{16}$$

Similarly from (13), can be deduced

$$\begin{aligned}&\int_0^T-\langle\mathbf{v}',\mathbf{u}_m\rangle+F[\mathbf{u}_m,\mathbf{v};t]dt\\&=\int_0^T(\mathbf{f},\mathbf{v})dt+(\mathbf{u}_m(0),\mathbf{v}(0))\end{aligned}$$

Set $m=m_l$ and once again employ (11) to find

$$\int_0^T-\langle\mathbf{v},\mathbf{u}\rangle+F[\mathbf{u},\mathbf{v};t]dt=\int_0^T(\mathbf{f},\mathbf{v})dt+(g,\mathbf{v}(0))\tag{17}$$

since $u_{ml}(0)\to g$ in $L^2(U)$. As $\mathbf{v}(0)$ is arbitrary, comparing (16) and (17), lead to $\mathbf{u}(0)=g$.

Also a weak solution of (1) is unique. For this purpose, it suffices to check that the only weak solution of (1) with

$f = g = 0$ is $\mathbf{u} \equiv 0$. To this, observe that by setting $\mathbf{v} = \mathbf{u}$ in identity (15) (for $f = 0$),

$$\frac{d}{dt}\left(\frac{1}{2}\|\mathbf{u}\|^2_{L^2(U)}\right) + F[\mathbf{u},\mathbf{v};t] = (\mathbf{u},\mathbf{u}) \qquad (18)$$

Then Gronwall's inequality

$$F[\mathbf{u},\mathbf{u};t] \geq \beta\|\mathbf{u}\|^2_{H^1_0(U)} - \gamma\|\mathbf{u}\|^2_{L^2(U)} \geq -\gamma\|\mathbf{u}\|^2_{L^2(U)}$$

and (18) imply $\mathbf{u} \equiv 0$.

For the last assertion of the theorem, suppose $V \subset \overline{V} \subset U$ and $\overline{V}$ is compact and connected. Then there exists a constant c such that the Harnak's inequality $\operatorname{Sup}_V u(.,t_1) \leq c \inf_V u(.,t_2)$ is established for each $0 < t_1 < t_2 \leq T$.

The constant c depends only on V, t_1, t_2 and the coefficient of P (of course, if the coefficients are continuous or bounded, it is manageable, too).

In this way, Harnack's inequality states that if u is a nonnegative solution of the parabolic PDE (1), then the maximum of u in some interior at a positive time can be estimated by the minimum of u in the same region at a later time.

Of course, SSF bioreactors have these features geometrically and all the equations in Table 1 have these conditions, therefore, their diffusion will be controlled by this method.

The steps of the proof steps can be summarized in Figure 1.

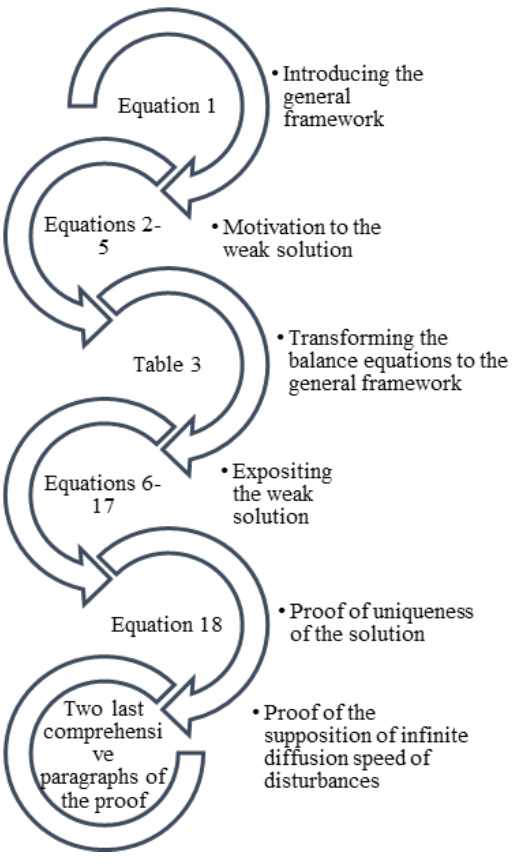

Figure 1. Structure of the Proof of Theorem

4. Conclusions

In this paper, a new method for obtaining the solution of oxygen balance equations, water balance and energy balance equations for bioreactors are presented. The proposed approach was based on the advanced concepts of functional analysis, such as the Sobolev spaces and weak solutions which led to the simplification of the problem and the reduction of partial differential equations into ordinary differential equations. In fact, Galerkin method convert the differential equation, in a weak formulation, to a discrete problem by applying linear constraints determined by finite sets of basis functions. The proof-of-process also lead to show that the approach offered was of the best kind and the weak solution is the best one in this structure.

One of the advantages of the proposed method can be well outlined in its superiority to the numerical methods used for these important problems of mass and heat transfer. The other benefit is that it supports infinite diffusion speed of disturbances. Then can be suitable for heat and mass–transfer models in (semi-infinite) SSF bioreactors with more diffusion.

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