Chapter 5

Modeling and simulation of temperature gradients in packed bed solid state fermenter
CHAPTER – 5

MODELING AND SIMULATION OF TEMPERATURE GRADIENTS IN PACKED BED SOLID STATE FERMENTER

ABSTRACT:

Modeling of solid state fermenter plays a vital role in understanding the bio process, design and development. Packed bed solid state fermenter (PBSSF) showed certain specified application over another types of SSF. Overall efficiency of this reactor majorly depends on the temperature gradients formed inside the column and hence in this research work, kinetic and lumped heat transport model were used for simulating the microbial growth in the PBSSF. Aspergillus oryzae was grown on JS and then experimental findings were validated by checking its fitness with the lumped model and found to be satisfactory.

Keywords: Modeling; PBSSF; initial biomass; true density.

5.1 Introduction:

Solid-state fermentation (SSF) involves the growth of microbes, mostly fungi on water insoluble substrates in the absence of free water[1]. SSF is a very complex process where precise monitoring of process variables and controlling is required. Efficiency of SSF processes depends on interface between the three key components of the system: The bioreactor, the substrate and the micro-organisms used.[2,3] During the latest decade, SSF has experienced renewed interest due to many potential advantages of this bioprocess in
comparison with submerged fermentation (SmF). These advantages include smaller bioreactor volumes, reduced downstream processing costs, superior productivity, simpler techniques, reduced energy requirements and low wastewater output\[^{4,22}\]. SSF shows its fundamental ability to utilize insoluble solid substrate efficiently. However, solid medium poses problems related to mass and heat transfer which becomes a major hurdle in applicability of SSF. When compared with other types of SSF, PBSSF shows better process economics and even loading and unloading is easy in PBSSF. PBSSF is a cylindrical vessel with perforated base and hemispherical head. Although, PBSSF is very easy for fabrication, its process variables are very difficult to control. Larger bed heights accommodating high substrate volume are possible with PBSSF, in which air is spurge through the bottom of the bed\[^{5,7}\]. In PBSSF oxygen supply is not limiting due to continues gas phase\[^{8-9}\]. Temperature variation formed inside the column is very severe technical problem with PBSSF. These temperature variations inside the column effect on the growth of micro-organism. The kinetic model shows the effect of these temperature variations on micro-organism growth. Heat generated inside the column can be largely dissipated by forced aeration and little bit by conduction mechanism which creates high temperature at the top of the column\[^{24}\]. Bathe *et al.*, \[^{10}\] experimentally found that JS substrate C:N ratio was found to be > 18 and hence it is suitable substrate for SSF. In the current work, temperature variations were studied for the growth of *Aspergillus oryzae* on JS.
5.2 Materials and Method

5.2.1 Experimental Set-up:

The experimental setup of a PBSSF is shown in Fig. 5.1. It consists of a cylindrical unit (1) with a capacity of 11.9 litres. It was 42 cm long vertical cylinder with internal diameter of 19 cm. The material used for the construction of fermentor system is SS-304. The base of fermentor was made up of wire mesh (2) with air distributor to facilitate aeration. The packed bed was aerated through air filter with a constant velocity of 60 m/hr. The bed temperatures were measured by thermocouple PT100 (3) placed at different axial positions and recorded by a data acquisition system (4).

![Diagram of PBSSF](image)

**Fig.5.1** SS-304 Packed-bed solid state fermenter (PBSSF): (1) Fermentation vessel, (2) Air distributor plate, (3) PT100 thermocouple, (4) Data acquisition system.
5.2.2 Pretreatment of raw material

The measured quantity of JS was crushed in the mixer and screened to a mesh size of 36 for its utilization. The material was mixed with water and resulting thick slurry was pretreated in an autoclave for 0.5 hr at 1 bar. The mixture was gradually allowed to cool down to ambient temperature and then dried in a convection oven to maintain overall moisture content in the range of 60% - 65%.

5.2.3 Inoculum preparation

The spores of a fungus Aspergillus oryzae were inoculated in Czapek Dox broth having sucrose as carbon source and incubated for 48 hours at 30°C. After incubation, 5% v/w inoculum was inoculated in the pretreated substrate.

5.2.4 Material properties

Bulk properties of the packed bed of substrate, like porosity, true density and bulk density were determined using pycnometer. Crushed JS was pretreated with distilled water for 15 min and dried overnight. It was the filled in the pycnometer. The volume of toluene required to fill up all pores (spaces between two adjacent particles) was measured. Based on experiments, true and bulk properties were determined as follows.

5.2.4.1 Bed porosity

Bed porosity(ε) of the substrate was calculated using following equation

\[ \varepsilon = \left(1 - \frac{\rho_b}{\rho_t}\right) \]  

Where, \( \rho_b \) is bulk density and \( \rho_t \) is true density of the bed.

Volume was calculated by following relationship
\[ V = \frac{(M_{ps} - M_p) - (M_{pts} - M_T)}{\rho_{tol}} \] \hspace{1cm} \text{(ii)}

Where \( M_T \) is mass of the pycnometer filled with toluene, \( M_{ps} \) is the mass of pycnometer and sample, \( M_p \) is the mass of the pycnometer, \( M_{pts} \) is the mass of the pynometer filled with toluene and the sample and \( \rho_{tol} \) is the density of toluene. After calculating volume(V), true density then can be calculated by following relation

\[ \rho_t = \frac{(M_{ps} - M_p)}{V} \] \hspace{1cm} \text{(iii)}

### 5.2.5 Initial biomass formed

Biomass is a very essential parameter for characterizing the fungal growth and is necessary for measuring growth kinetics in SSF\textsuperscript{[23]}. To find the initial biomass it was filtered from inoculum and washed thoroughly with de-ionized water and dried in tray dryer at 60\(^\circ\)C for 48 h. Dried biomass was weighed at a regular interval of time (2h) for 48 h. The constant weight value between 4 successive intervals was considered as final biomass concentration.

### 5.3 Mathematical model

In spite of mathematical simplicity with many unstructured models, they predict only adequate approximation of the whole growth curve in terms of three stages including the lag, exponential growth and stationary phases and exclude complete representation of the death phase \textsuperscript{[14]}. In the present study, the growth kinetics of \textit{Aspergillus oryzae} on JS in the batch bioreactor was correlated with temperature rate to predict behavior during lag, exponential growth stationary phases with an emphasize on death phase. The models
describing interrelation of growth rate to the reactor temperature have already been devised as kinetic and transport models. The lumped model approach followed by Fanaei and Vaziri \cite{14} has been used to investigate growth kinetics and heat transfer dynamics. Kinetic models describe how the microorganisms are influenced by various process parameters while transport model describes the mass and temperature profiles within the packed-bed bioreactor systems. In the current work, the model developed by Fanaei and Vaziri best fitted for the experimental data generated when *Aspergillus oryzae* was grown on JS.

### 5.3.1 Kinetic model

The parameter values used in the kinetic and lumped heat transfer model are given in Table 5.1 \cite{14,15,17,19}. Growth kinetics model for *Aspergillus oryzae* on JS is as follows:

\[
\frac{dx}{dt} = \mu \Phi X (1 - \frac{X}{X_m}) \tag{iv}
\]

Where, \(X, X_m\) and \(\Phi\) are the biomass concentration, the maximum biomass concentration and the level of a physiological factor respectively. Physiological factor signifies the physiological state of the organisms during the course of fermentation and is function of temperature. Its value remains approximately equal to 1 during the biomass growth which indicates that is effect on growth in negligible in the temperature range selected. \(\mu\) is the specific rate constant and calculated from equation (vi).
5.3.2 Heat capacity of air (Cpa)

The heat capacity \[^{15}\] of air (J kg\(^{-1}\)°C\(^{-1}\)) at 30 °C was calculated using correlation

\[
C_{pa} = 997.9 + 0.143 \, T - 0.00011 \, T^2 - 6.776 \times 10^{-8} \, T^3 \quad \text{…………..(v)}
\]

Where, \(C_{pa}\) is heat capacity of air and \(T\) is inlet air temperature.

5.3.3 Specific growth rate constant

It was calculated by following relation\[^{16}\]

\[
\mu = \left( \frac{s + (T_{max} - T_{opt})}{T_{max} - T_{opt}} \right) \left( \frac{\mu_{opt} + (T_{max} - T)}{s + (T_{max} - T)} \right) \quad \text{………………………….(vi)}
\]

Where, \(s\) is the sensitivity of the specific growth rate, \(T_{max}\) and \(T_{opt}\) are the maximum and optimum temperatures for micro-organism growth and \(\mu_{opt}\) is the optimum specific growth rate constant.

5.3.4 Dynamic heat transfer models:

Lumped dynamic heat transfer model expressed\[^{14}\] as follows

\[
\rho_b C_{pb} \left( \frac{\partial T}{\partial t} \right) = \rho_s (1-\epsilon) \, Y_0 \frac{dx}{dt} + \rho_s C_{pav} \frac{V_H}{H} (T_a - T) + \rho_s \rho \frac{V_H}{H} (T_a - T) \quad \text{……..(vii)}
\]
Table 5.1 Parameter values used in the simulations with the mathematical model

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Explanation</th>
<th>Value</th>
<th>Method used</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>Bed height (temp. sensor placed at this height)</td>
<td>0.25m</td>
<td>Exp. Reading</td>
</tr>
<tr>
<td>ε</td>
<td>Porosity</td>
<td>0.8367</td>
<td>Exp. Calculated</td>
</tr>
<tr>
<td>To</td>
<td>Bed temperature</td>
<td>30 °C</td>
<td>Exp. Reading</td>
</tr>
<tr>
<td>Ta</td>
<td>Inlet air temperature</td>
<td>29.6 °C</td>
<td>Exp. Reading</td>
</tr>
<tr>
<td>ρs</td>
<td>Substrate density</td>
<td>710 Kg m⁻³</td>
<td>Exp. Calculated</td>
</tr>
<tr>
<td>X₀</td>
<td>Initial biomass</td>
<td>0.0025</td>
<td>Exp. Calculated</td>
</tr>
<tr>
<td>1/Xm</td>
<td>Maximum possible biomass concentration(Xm)</td>
<td>5.8824</td>
<td>Fitting of experimental data</td>
</tr>
<tr>
<td>Tmax</td>
<td>Maximum Temperature for growth</td>
<td>44 °C</td>
<td>Exp. Finding</td>
</tr>
<tr>
<td>Topt</td>
<td>Optimum temperature for growth</td>
<td>30 °C</td>
<td>Exp. Finding</td>
</tr>
<tr>
<td>V_H</td>
<td>Velocity of moist air</td>
<td>60 m hr⁻¹</td>
<td>Exp. Value</td>
</tr>
<tr>
<td>K_s</td>
<td>Thermal conductivity of substrate</td>
<td>1080 J hr⁻¹ m⁻¹ °C⁻¹</td>
<td>Assumed</td>
</tr>
<tr>
<td>K_a</td>
<td>Thermal conductivity of moist air</td>
<td>74.16 J hr⁻¹ m⁻¹ °C⁻¹</td>
<td>[17]</td>
</tr>
<tr>
<td>f</td>
<td>Water carrying capacity of air</td>
<td>0.002496kg-water/air⁻¹ °C⁻¹</td>
<td>[17]</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Value</td>
<td>Source</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
<td>------------------------</td>
<td>--------</td>
</tr>
<tr>
<td>S</td>
<td>Sensitivity of the specific growth rate to increases in temperature</td>
<td>6.275</td>
<td></td>
</tr>
<tr>
<td>α</td>
<td>Exponent in the power law version of the logistic equation</td>
<td>11 (dimensionless)</td>
<td>[14]</td>
</tr>
<tr>
<td>φ</td>
<td>Level of a physiological factor</td>
<td>1</td>
<td>[14]</td>
</tr>
<tr>
<td>µ</td>
<td>Specific growth rate constant</td>
<td>h⁻¹</td>
<td></td>
</tr>
<tr>
<td>µₜₒₜₜ</td>
<td>Optimum specific growth rate constant</td>
<td>0.122 h⁻¹</td>
<td></td>
</tr>
<tr>
<td>ρₐ</td>
<td>Moist air density</td>
<td>1.14 kg m⁻³</td>
<td>[15]</td>
</tr>
<tr>
<td>λ</td>
<td>Latent evaporation of water</td>
<td>2414300 J kg-water⁻¹</td>
<td>[15]</td>
</tr>
<tr>
<td>Cₚₐ</td>
<td>Heat capacity of air</td>
<td>1002.07 J kg⁻¹°C⁻¹</td>
<td>Calculated by eq.(5)</td>
</tr>
<tr>
<td>Cₚₛ</td>
<td>Heat capacity of substrate</td>
<td>2500 J kg⁻¹°C⁻¹</td>
<td>Assume data</td>
</tr>
<tr>
<td>Yₒ</td>
<td>Metabolic heat yield coefficient</td>
<td>8.366*10⁶ J kg⁻¹ biomass⁻¹</td>
<td>[19]</td>
</tr>
</tbody>
</table>
5.4 Results and Discussion:

In the present study, it was assumed that the growth kinetics was carried out at the optimum water activity for growth and the effect of moisture content on growth was negligible. The experimental data used in this investigation were determined by lab experiments. The values of few parameters like porosity, substrate density, true density, initial biomass generated by experiments are given in Table 5.2.

Table 5.2 Fermentation parameters determined

<table>
<thead>
<tr>
<th>Sr.No.</th>
<th>Parameter</th>
<th>Symbol</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Porosity</td>
<td>$\varepsilon$</td>
<td>0.8367</td>
</tr>
<tr>
<td>2</td>
<td>Substrate density</td>
<td>$\rho_s$</td>
<td>710 Kg/ m³</td>
</tr>
<tr>
<td>3</td>
<td>True density</td>
<td>$\rho_t$</td>
<td>0.6168 gm/cm³</td>
</tr>
<tr>
<td>4</td>
<td>Initial biomass</td>
<td>$X_0$</td>
<td>0.0025 kg of biomass/ kg of substrate</td>
</tr>
</tbody>
</table>

The optimum temperature for the growth of *Aspergillus oryzae* is 30°C. The experimental data was generated to fit the heat transfer models in a SSF process. The fermentor used in this work was a SS-304, packed bed column with 42 cm height and 19 cm diameter. This fermenter was aerated from the bottom. Temperature variation profiles were reported at 25 cm height and therefore, same height was used as a fermenter height in the simulation. Fig.5.2 shows the predictions of lumped heat transfer model (temporal temperature
profiles) with the experimental results. The results show that the predictions of lumped model are in good agreement with experimental data. The average of sum squared error (SSE) for predictions of lumped model is 4.67.

Fig.5.2 Comparison of the predictions of lumped heat transfer model with experimental data

Specific growth rate constant $\mu$ is a function of temperature. Growth rate of synthesis reaction and denaturation reaction is shown in Fig.5.3. In PBSSF heat is mainly transferred by convective mode. Fig.5.4 indicate the biomass growth curve which shows the lag phase upto 20 h then during the period 20 h to 45 h exponential phase was observed and above 45 h to 65 h stationary phase was observed. After 45 h growth curve
slope decreases because at this time temperature rich to high reading affect spore germination and growth. Hence, after 45 h temperature was observed to be almost constant up to 65 h indicates stationary phase as shown in Fig.5.2. As after 65 h the temperature was observed to be decreased due to spore germination and decrease in the growth rate indicated death phase.

Fig.5.3: Specific growth rate versus bed temperature
According to Mitchell et al.,\cite{20,21} temperature gradients forms in PBSSF are impossible to avoid and sometimes these gradient may be steep due to the end to end aeration. Between the time 20 to 45 h the temperature gradients were steep. These results showed that between this time period metabolic activities of the micro-organism were very high which generated heat.

Numerical solution of the kinetic and heat transfer models were performed by the STIFFBS method in Polymath 6.1- educational version, with the regression coefficient ($r^2$) of 0.997. This value of $r^2$ shows that the lumped model was effectively fitted to experimental data. To verify the validity of kinetic model proposed by Fanaei and Vaziri, experimental data generated for the growth of \textit{Aspergillus oryzae} on JS was used.

**Fig5.4: Growth of \textit{Aspergillus oryzae} on JS**
results are shown in Fig.5.4. From these results, the model predictions agreed reasonably well with the experimental data.

5.5 Conclusions:

In the present study, the growth kinetics of Aspergillus oryzae on JS in the batch bioreactor was correlated efficiently with temperature rate to predict behavior during lag, exponential growth stationary phases with an emphasize on death phase. Kinetic and lumped heat transfer models were tested for PBSSF and were in agreement. Experimental data of temperature variation fitted perfectly with this model. This model used the novel approach of the influence current temperatures on growth phases. An attempt is made to completely represent the death phase using relationship between specific rate constant and temperature.

Nomenclature

Cpa  Heat capacity of air (J/kg °c)
Cps  Heat capacity of substrate (J/kg °c)
f    Water carrying capacity of air (kg-water/kg-air °c)
H    Bed height (m)
Ka   Thermal conductivity of moist air (J/hr m °c)
Ks   Thermal conductivity of substrate (J/hr m °c)
t    Time (hr)
T    Bed temperature (°c)
To   Initial bed temperature (°c)
Ta   Inlet air temperature (°c)
Tmax Maximum Temperature for growth (°c)
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Topt  Optimum temperature for growth (°C)

V_H  Velocity of moist air (m/hr)

X  Biomass concentration (kg-biomass/kg-substrate)

X_0  Initial biomass concentration (kg-biomass/kg-substrate)

X_m  Maximum biomass concentration (kg-biomass/kg-substrate)

Y_Q  Metabolic heat yield coefficient (J/kg-biomass)

H  Axial position

H  Bed height (m)

Greek letters

ߝ  Porosity

λ  Latent evaporation of water (J/Kg)

µ  Specific growth rate constant (hr⁻¹)

µ_{opt}  Optimum specific growth rate constant (hr⁻¹)

ρ_a  Moist air density (kg/m³)

ρ_s  Substrate density (kg/m³)

ρ_t  True density (kg/m³)
STIFFBS method programme in Polymath 6.1- educational version

POLYMATH Results
No Title 01-26-2013, Rev5.1.233

Calculated values of the DEQ variables
Variable initial value minimal value maximal value final value
T 0 0.120 120
X 0.0025 0.0025 0.1699168 0.1699168
T 30 29.629562 39.172301 29.629562
phi 1 0.9925802 1 0.9968655
A 0.83 0.83 0.83 0.83
B 1.14 1.14 1.14 1.14
C 710 710 710
D 74.16 74.16 74.16 74.16
E 1080 1080 1080 1080
F 1180 1180 1180 1180
G 0.002496 0.002496 0.002496 0.002496
H 2.414E+06 2.414E+06 2.414E+06 2.414E+06
I 2500 2500 2500 2500
J 44 44 44 44
K 30 30 30 30
L 0.115 0.115 0.115 0.115
M 5.8824 5.8824 5.8824 5.8824
N 8.366E+06 8.366E+06 8.366E+06 8.366E+06
O 29.6 29.6 29.6 29.6
P 60 60 60 60
Q 0.25 0.25 0.25 0.25
S 6.275 6.275 6.275 6.275
V 0.25 0.25 0.25 0.25

ODE Report (STIFFBS)
Differential equations as entered by the user
[1] \frac{d(X)}{dt} = \frac{(L^*(S+J-K)*(J-T)*(1-(M*X))*phi*X)((S+J-T)*(J-K))}{((S+J-T)*(J-K))}
[2] \frac{d(T)}{dt} = \frac{(C*(1-A)*N)*(L^*(S+J-K)*(J-T)*(1-(M*X))*phi*X)((S+J-T)*(J-K))+(B*F*(P/Q)*(O-T))+(B*G*H*(P/V)*(30-T)))}{((A*B*(F+(G*H)))+(C*I*(1-A)))}
[3] \frac{d(phi)}{dt} = \frac{(9.761*(10^8)*phi*(1-(phi^11)))*exp(-8195.071/(T+273))-(8.74*(10^45)*phi*exp(-35421.931/(T+273)))}{O-35421.931/(T+273))}

Explicit equations as entered by the user
[1] A = 0.83
[3] C = 710
[4] D = 74.16
[5] E = 1080
[6] F = 1180
[7] G = 0.002496
[8] H = 2414300
[9] I = 2500
[10] J = 44
[12] L = 0.115
[15] O = 29.6
[16] P = 60
[17] Q = 0.25
[18] S = 6.275
[19] V = 0.25
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initial value : 0
final value : 120
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Minimum allowed stepsize. hmin = 0.00001
Good steps = 284
Bad steps = 467
General
number of differential equations: 3
number of explicit equations: 19
Elapsed time: 8.1019 sec
Data file: E:\Local Disk D\Bathe Sir Modeling\Bathe sir modified.pol
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References:


