VALIDATION OF CFD MODEL AND DECIPHERING THE BEHAVIOR OF PACKED BED REACTOR BY COMPARATIVE TECHNIQUE OF RTD AND CFD

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ABSTRACT
Water is one of the greatest essences in today’s world. Treatment of waste water could solve a lot of problems faced by modern world. Motive of this study is to treat industrial waste water. We know that to treat industrial waste water packed bed bioreactors are installed in some of the industry. In the present study, to understand performance of reactor we did develop a CFD model. By observing change in conductivity of tracer solution we measure the values of experimental RTD. Then solution for transport equation for geometrical configuration of a reactor is found via CFD simulation. The result obtained by CFD simulation & experimental value of RTD were compared to have a better design and to find out optimum conditions of a packed bed reactor. Experimental results are in hand-to-hand with those of CFD simulation.

KEYWORDS: Residence Time Distribution (RTD), Computational Fluid Dynamics (CFD), Packed Bed Reactor, Tracer Testing, Simulation.

1. INTRODUCTION
From a last few decades, packed bed bioreactors are used for the treatment of biological waste water. In chemical engineering field, residence time distribution (RTD) of a chemical reactor is a probability distribution function that describes the amount of time a fluid element could spend inside the reactor taking different routes and different lengths.¹[1] RTD provides
information about material flow in many continuous flow processes which have a wide use in industries. Thus, we got a very efficient tool in form of analysis of RTD to check out feasibility of chemical reactors. The injected inert chemical, molecule, or atom, called a tracer, chosen to follow the evaluation of RTD in bioreactors for fixed biomass is decisive. There are many type of tracer detection technique, but here we used two of them namely Inline and Offline. In inline detection technique, the system is unsettled by using either a pulse or a step input in form of thermal or electrical signal and then records directly from inline probes how the system responds to this input. When these steps cannot be finished instantly usage of Offline detection is preferred. Here optical and conductivity method are used for tracer detection. Usage of different types of dyes as tracer compounds has been reported in literature. Different criteria like solubility, adsorption on biomass, pH stability and time stability were considered to select suitable dye tracer. In various studies different dyes which are not harmful for laboratory purpose like brome cresol green, brome phenol blue, dextrin blue 2000, eosin y, mordant violet, ethylene violet, ethylene blue, rhodamine b and brilliant green have been used. Among the above mentioned dyes brome cresol green, brome phenol blue, dextrin blue 2000, eosin y and mordant violet provides good solubility, no adsorption on biomass, stability in time and no color change between ph 6.5 to 8.5. To determine RTD experimentally, the tracer material is injected at input and the response of tracer profile is recorded at outlet of the system. Stimulus response is the most common method used for measurement of RTD. Stimulus response is an inline detection technique so tracer is injected in the form of pulse input, step input, square pulse, Ramp input and sinusoid input. Mostly used inputs for the measurement of RTD are step and pulse input. These two methods are used in this study too. In step input the tracer is added along with the feed at a constant rate whereas in pulse input, a small, known amount of tracer material is injected by a syringe.

Reactor’s performance can be simulated by different models, major among which are Dispersion model, plug flow model, distribution flow model, laminar flow model and much more. In the present study, two methods namely Residence Time Distribution (RTD) experimental technique and Computational fluid Dynamics (CFD) simulation are used for understanding the behavior of packed bed reactor. RTD experimental tracer results must validate the outcome of Computational fluid Dynamics (CFD) model results. CFD is a numerical simulation method for analysis of industrial complex processed whereas RTD is a
completely experimental method. Both RTD and CFD are suitable methods for analysis of flow system in industrial processes.

It is crucial to develop a CFD model and utilize its feasibility for design of industrial systems. Before they are applied to industrial systems we need to verify these CFD models to provide reliable and accurate results. In order to verify these CFD models the CFD model results should be supported with RTD experimental results.

2. MATERIALS
- Milipore water (R=18.2M Ω·cm)
- Tracer solution of conc. sulphuric acid
- N/10 NaOH
- Phenolphthalein
- conductivity meter (HACH)

All the experiments were performed at room temperature (298K).

3. METHODS

Table: 1 Salient feature of Bio-column Reactor

<table>
<thead>
<tr>
<th>SR No</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Diameter of reactor (cm)</td>
<td>8.0</td>
</tr>
<tr>
<td>2</td>
<td>Total height of reactor (cm)</td>
<td>100</td>
</tr>
<tr>
<td>3</td>
<td>Volume of reactor (liters)</td>
<td>5.03</td>
</tr>
<tr>
<td>4</td>
<td>Number of sampling point (cm)</td>
<td>5.0</td>
</tr>
<tr>
<td>5</td>
<td>Height of sampling point (cm)</td>
<td>100</td>
</tr>
<tr>
<td>6</td>
<td>Diameter of sampling point (cm)</td>
<td>1.25</td>
</tr>
<tr>
<td>7</td>
<td>Total Weight of Absorbent (gm)</td>
<td>2420</td>
</tr>
<tr>
<td>8</td>
<td>Density of Bed (gm/mL)</td>
<td>0.7166</td>
</tr>
<tr>
<td>9</td>
<td>Actual Volume of Reactor (Liters)</td>
<td>1.623</td>
</tr>
</tbody>
</table>

3.1 Experimental setup: In a packed bed bioreactor response of RTD experiments were carried out. The schematic diagram of experimental setup, which consists of packed bed bioreactor, injection point, mixing tank fitted with stirrer (feed chamber), peristaltic pump, filter unit for water, pressure gauge, level indicator, and sampling port is shown in Fig 1. The reactor was made up of SS 316 (Stainless Steel 316) with an inner diameter 8 cm, height 100 cm and working volume of 5.02 L. The reactor was filled with java plum core/seed of particle size of 2-6 mm and bulk density of 71.66g/100ml. The reactor assembly was a close circuit unit. Five equidistant ports (P1, P2, P3, P4, P5) of 1.25 cm diameter were equipped for
collecting liquid samples along the height of the reactor. The final pore volume (void space) of the reactor with java plum core/seed packed bed reactor was between 1300-1400 ml.

![Experimental Setup for RTD](image)

**Fig. 1 Experimental Setup for RTD**

3.2 Spectrophotometric methods: In this technique, a compound of a metal such as aluminium, iron, thorium, zirconium, lanthanum or cerium reacts with an indicator dye to build a complex of small dissociation constant. This complex reacts with fluoride to give a new complex. Because of the transformation in the configuration of the complex, the surface assimilation spectrum also shifts relative to the spectrum for the fluoride-free reagent solutions. This alteration can be observed by using a spectrophotometer. One of the essential dyes employed is trisodium 2-(parasulfophenylazo)-1, 8-dihydroxy-3, and 6-naphthalene disulfonate, generally recognized as SPADNS. Erichrome Cyanine R is one more usually used dye. The dye reacts with metal ions to give a coloured complex. In the SPADNS method, zirconium reacts with SPADNS to build a red coloured complex. Fluoride discolours the red colour of the complex and therefore the alteration in absorbance can be calculated using a spectrophotometer.

![Formation of the SPADNS – ZrOCl2 complex](image)
3.3 Procedure
In this experiment we first close the drain valve provided at the bottom of the feed tank to fill it with water. When the feed tank is filled with water a injection containing 20 ml conc. H₂SO₄ is placed at the tracer injecting point after opening the dead end. Once it is ensured that knob provided on the pumps is at zero position, Set rotation selection switch towards clockwise rotation arrow while Set other switch provided on the pump towards Manual option. When the flow rate gets stabilised, inject quickly the pulse tracer from the syringe. Start the stop watch simultaneously. Collect 10 ml of exit stream sample from the top at 0.5 min interval. Take the sample and titrate with N/10 NaOH using phenolphthalein as the indicator.

3.4 Reactions Involved
- H₂SO₄ + 2 NaOH → Na₂SO₄ + 2H₂O
  Or
- HCl + NaOH → NaCl + H₂O

4. RESULTS AND DISCUSSION
In This section we discussed results obtained by that of the experimentally measured RTD and RTD validation by CFD model. A numerical experiment was performed by using the computational fluid dynamic (CFD) for the evaluation and validation by RTD experimental technique. RTD analysis was carried out by performing tracer experiment in laboratory scale. Here we used CFD code FLUENT to obtain a solution.

4.1 Axial Dispersion model
For CFD modelling mass and momentum equations were solved using numerical techniques. Since these equations cannot be solved analytically therefore they were linearized and solved...
by computational mesh.

The dispersion model is presented in form of differential equation by a single one dimensional Fick’s law mechanism:

\[
\frac{1}{P_e} \frac{d^2 c}{dx^2} - \frac{dc}{dx} - \frac{dc}{d\theta} = 0
\]  

(1)

The dispersion model contains only one parameter as Peclet number \((P_e)\). For high dispersion the equ-1 can be solved as

\[
E_{\theta} = \sqrt{\frac{P_e}{4\pi \theta}} \exp\left[-\frac{P_e}{4\theta} (1-\theta)^2\right]
\]  

(2)

The tracer study methodology was used to obtained Experimental RTD for both Step and pulse input by plotting graphs between \(E_{\theta}\) & \(\theta\)

Various parameters used in RTD evaluation are calculated using following equations:

\[
\sigma^2 = \int_0^\infty (t - \tau)^2 \ E(t) \ dt
\]  

(3)

\[
\theta = \frac{\tau}{\bar{\tau}}
\]  

(4)

4.2 Comparative analysis of Experimental and Simulated RTD

![Graph showing CFD simulated and experimentally measured dimensionless RTD for step change](image)

Fig 2. CFD simulated and experimentally measured dimensionless RTD for step change

Fig 2 demonstrates E graph of pulse and step input method respectively. It can be observed
from fig 2 that the CFD simulated RTD very closely matches with Experimentally RTD for both step and pulse input. The comparison between the experimentally RTD and simulated RTD are presented in table 1. It can be observed from Table 1 that Variance \( \sigma^2 \), Mean residence time \( \tau_m \) and Peclet number of experimental and simulated RTD are in close proximity. The validation results show that the CFD model is able to accurately predict the RTD.

Table 2: Comparison between Experimental Residence Time Distributions for packed bed reactor and Computational Fluid dynamics model Residence Time Distribution.

<table>
<thead>
<tr>
<th>Residence Time Distribution measure</th>
<th>( \sigma^2 )</th>
<th>( P_e )</th>
<th>( \sigma^2 )</th>
<th>( \tau_m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Computational Fluid dynamics simulated Residence Time Distribution for step Change</td>
<td>240.1136</td>
<td>23.167</td>
<td>0.1103</td>
<td>13.65</td>
</tr>
<tr>
<td>Experimental Residence Time Distribution For step change</td>
<td>242.1136</td>
<td>22.167</td>
<td>0.1065</td>
<td>12.564</td>
</tr>
</tbody>
</table>

5. CONCLUSIONS

In present study, Residence Time Distribution for packed bed reactor for step input change was investigated experimentally. Simulation result for step input was in good agreement with experimental results. Residence Time Distribution method provide a useful tool for efficient operation design and system improvement. The variance \( \sigma^2 \), Mean residence time \( \tau_m \) and Peclet number of experimental and simulated Residence Time Distribution are provide close approximately. The validation results show that the Computational Fluid dynamics model is able to accurately predict the Residence Time Distribution.

REFERENCES

