Distribution of RTD in Liquid Phase in Packed Column and CFD Model Validation

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Abstract—Packed bed bioreactors have been successfully used in treatment of industrial wastewater. In this study a CFD model was developed to understand reactor performance. Experimental RTD measurement was performed by monitoring the conductivity of tracer solution. The transport equation for geometrical configuration of a reactor is solved by CFD simulation and model results are compared with RTD experimental tracer results. A comparison between model results and experimental results provides the potential role for design and determination of operating condition of a packed bed reactor. The CFD simulation shows a good agreement with experimental results.

Keywords—Computational Fluid Dynamics, Residence Time Distribution, Tracer Testing, Simulation, Packed bed Reactor.

I. INTRODUCTION

Packed bed bioreactors have been used in treatment of biological waste water from last few decades. In chemical engineering field RTD, residence time distribution, is defined as the fluid element passing through the reactor, taking different routes and different lengths of time to pass through the reactor (3). RTD also provides information about material flow profile in many industrial continuous flow processes. The analysis of RTD is a very useful evaluation tool for inspection of feasibility of chemical reactors. The selection of tracer used for evaluation of RTD in bioreactors for fixed biomass is important. Two types of trace detection technique have been used: inline and offline. In inline detection technique thermal or electrical signal of tracer concentration is directly recorded from inline probes [12]. Offline detection is used when these steps cannot be finished instantly [2, 7, 8, 10]. Two method used for such tracer detection are optical and conductivity [5, 11, 13]. Use of different types of dyes as tracer compounds have been reported. For selection of dye as tracer different criteria have to be noticed like pH stability, solubility, time stability and adsorption on biomass. Different dyes (colorant) like brilliant green, bromocresol green, bromophenol blue, mordant violet, dextran blue 2000, eosin y, methylene blue, methylene violet and rhodamine b, which are not harmful for laboratory purpose, have been used in various studies (6). Among them bromocresol green, bromophenol blue, dextran blue, eosin y, and mordant violet provide good solubility, no adsorption on biomass, stability in time and no color change between pH 6.5 to 8.5 (6). For determination of RTD the tracer material is injected at input and the response of tracer profile is recorded at outlet of the system. The most common method for measurement of RTD is stimulus response. The tracer can be injected by many types such as pulse input, step input, square pulse, Ramp input and sinusoid input. Mostly step and pulse input are used for the measurement of RTD. In pulse input, a small, known amount of tracer material is injected by a syringe whereas in step input the tracer is added along with the feed at a constant rate. The step and pulse test methods are used in this study. Reactor's performance may be simulated by different models as plug flow model, dispersion model, laminar flow model and distribution flow model etc. In this present study two methods are used for understanding the behavior of packed bed reactor, Residence Time Distribution (RTD) experimental technique and CFD simulation. Computational Fluid Dynamics (CFD) model results have to be verified by RTD experimental tracer results. RTD is an experimental method whereas CFD is a numerical simulation method for analysis of industrial complex processes. RTD and CFD both are suitable methods for analysis of flow system in industrial processes. It is necessary to develop a CFD model and utilize its feasibility for design of industrial systems and also need to verify these CFD models before they are apply for industrial systems to provide reliable and accurate results. So the CFD model results should be validated with RTD experimental results.
II. MATERIALS AND METHODS

A. Materials
Millipore water was with resistivity of 18.2M Ω-cm used in this study (Q-H₂O, Millipore Corp.). The tracer solution of potassium chloride (0.1 M)(Himedia) and 0.1% (w/w) Bromophenol blue(Himedia) was used for the analysis. Potassium chloride and Bromophenol blue both are environmentally safe. All the experiments were carried out at room temperature. A conductivity meter (HACH) was used for determination of performance of RTD experiment for both step and impulse input.

B. Experimental setup
RTD response experiments were carried in a packed bed bioreactor. The schematic diagram of experimental setup is shown in Fig 1., which consists of packed bed bioreactor, mixing chamber fitted with stirrer (feed tank), peristaltic pump, filter unit for water, level indicator, pressure gauge, injection point and sampling port. The reactor was made up of SS 316 (Stainless Steel 316) with an inner diameter 8 cm, height 100 cm and working volume of 5.01 l. The reactor assembly was a close circuit unit. Five equidistant ports 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 Rice husk packed bed reactor was between 2000-2100 ml.

C. Procedure
For concentration step change tracer experiment, the tracer solution of potassium chloride and Bromophenol was initially filled in the reactor. The purpose of Bromophenol is only give the color to the otherwise transparent solution. The step concentration test was performed by feeding Millipore water to the reactor with a constant flow rate of 10 lit/hr. The RTD was measured by conductivity of potassium chloride solution at the sampling port of the reactor at every 5 min interval. For pulse change flow of water was continued till steady state was attained after which 200 ml solution of potassium chloride and Bromophenol was injected in to the reactor through injection point. The conductivity of solution with respect to time was noted down at every 5 min interval.

III. RESULTS AND DISCUSSION
This section covers results and discussion of the experimentally measured RTDs and RTD validation by CFD model. A numerical experiment was performed by using the computational fluid dynamic (CFD) for the evaluation and validate by RTD experimental technique. RTD analysis was carried out by performing tracer experiment in laboratory scale. CFD code FLUENT was use to obtain a solution.

A. Axial Dispersion model
For CFD modeling 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:

\[
\frac{1}{P_e} \frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} + \frac{\partial c}{\partial \theta} = 0
\]

(1)

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

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

(2)

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

Various parameters used in RTD evaluation are calculated using following equations

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

(3)

\[
\theta = \frac{1}{\tau}
\]

(4)

B. Comparative analysis of Experimental and Simulated RTD
Fig 2 and 3 demonstrates E graph of pulse and step input method respectively. It can be observed from fig 2 and fig 3 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 (\(\sigma^2_{\theta}, \sigma^2\)), 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.
IV. CONCLUSIONS

In this study, RTD for packed bed reactor for step and impulse input were investigated experimentally. Simulation results for step and impulse input were in good agreement with experimental results. RTD method provide a useful tool for efficient operation design and system improvement. The variance ($\sigma^2$, $\bar{e}$), Mean residence time ($\bar{\tau}$) and Peclet number of experimental and simulated RTD are provide close proximity. The validation results show that the CFD model is able to accurately predict the RTD.

<table>
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<th>RTD measures</th>
<th>$\sigma^2$</th>
<th>$P_e$</th>
<th>$\bar{\tau}$</th>
<th>$\sigma^2$</th>
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<tr>
<td>CFD Simulated RTD for Step change</td>
<td>80.21</td>
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<td>Experimental RTD For Step change</td>
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REFERENCES