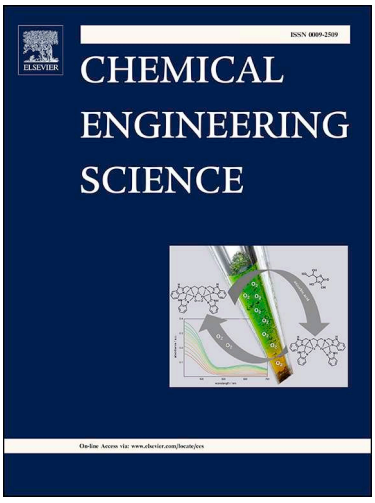

Gas phase dispersion/mixing investigation in a representative geometry of gas-liquid upflow moving bed hydrotreater reactor (mbr) using developed gas tracer technique and method based on convolution/ regression

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GAS PHASE DISPERSION/MIXING INVESTIGATION IN A REPRESENTATIVE GEOMETRY OF GAS-LIQUID UPFLOW MOVING BED HYDROTREATER REACTOR (MBR) USING DEVELOPED GAS TRACER TECHNIQUE AND METHOD BASED ON CONVOLUTION/ REGRESSION

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Abstract

Gas dispersion studies has been executed for the catalyst bed section of a representative geometry of scaled-down industrial Moving Bed Hydrotreater Reactor (MBR). The catalyst bed of MBR is modeled using Axial Dispersion Model (ADM) and its parameters gas dispersion coefficient (D_g) and peclet number (Pe) are estimated using Residence Time Distribution (RTD) and implementing a methodology based on convolution and regression. Additionally, dimensionless variance (σ_D^2) for the catalyst bed is also measured using RTDs first and second moments to compare with those findings of ADM model. This study is conducted at the varying flow rates of gas and liquid including scaled down operating conditions. The results of D_g, Pe, and σ_D^2 indicate that bed behaves as a packed bed for low liquid flow rate and moves towards three-phase fluidized bed for increasing liquid flow rate. Overall the gas phase behavior is seen to be in plug flow for all the operating conditions, with relatively high dispersion/mixing in packed bed state. Scaled down flow conditions is seen to be best in terms of gas dispersion/mixing and catalyst utilization.

Keywords: Residence Time Distribution (RTD), Moving Bed Reactor (MBR), Gas Tracer, Gas Dispersion Coefficient, Peclet Number, Axial Dispersion Model (ADM)

1. Introduction

Uplfow moving bed reactor is a hydrotreater and used for removal heavy metal content from crude oil. It is usually a replacement for fixed bed Hydrodemetalization reactor, which is guard reactor to the fixed bed residual desulfurization (RDS) unit [1]. This reactor has a catalyst bed section having a conical bottom and plena below the cone. The operating parameters are upflow movement of resid oil and hydrogen over hydrodemetalization catalyst (HDM), with flow conditions to limit the bed expansion to 10 percent of catalyst bulk volume [2] . The specialty of MBR is the conical bottom, which enables removal of spent catalyst under operation, this increases the run time of the reactor without shutdown. At industrial conditions, the catalyst removal takes place few times per week and that too in small increment, rest all time the reactor behaves as upflow packed bed or expanded bed. It is usually operated at a low linear velocity of the mixed feed to avoid substantial expansion (or contraction) of the bed [2]. The expanded bed or ebullated bed can improve the distribution of phases cross-sectionally but is usually not preferred due to increased catalyst attrition, bed mixing, increased reactor length for the desired conversion [2] at these conditions.

The major problems seen for this kind of reactor at industrial scale are catalyst coking, agglomeration, and early shutdown. The primary factors for these unwanted phenomena is maldistribution of phases [2] which can result in unwanted mixing behavior of phases or the coke reaction related to catalyst type and its reaction, which is the least studied reaction, but this study focus is mixing. The mixing of a phase within the reactor is conventionally classified as micromixing and macromixing [3]. Micromixing is the mixing occurring at the molecular level, and it depends on the intimacy of two nearby molecules. Micromixing parameter such as molecular diffusion is hard to estimate using experimental measurement technique. The macromixing phenomena is at a scale where the individual phase can be considered as an entity moving with convective dispersion and bulk flow and dispersing along axial, radial and angular direction. It is not feasible to measure the local velocity field profile at every possible local position within the reactor

to quantify macromixing. Therefore, RTD concept is used, where a tracer is injected and detected **at** the boundaries of test section and obtained RTD curve quantifies the dispserion/mixing in terms of its spread [4]. RTD's are comprehended using mass balance model having dispersion coefficient parameter, which lumps the non-ideality in terms of the convective dispersion and molecular diffusion, which dictates the spread in the RTD curve. Dispersion coefficient is an important design parameter, as the performance of any reactor depends on inter and intraparticle rate process for heat and mass transfer which is directly related to the mixing of phases. Hence, it is essential to determine the dispersion parameters and to integrate it with the intrinsic kinetics and other mass, and heat transfer parameters to yield reactor design and models, that account for certain extent of non ideality [3]. The knowledge of gas phase dispersion/mixing quantified in terms of dispersion coefficient is useful, as in most of the mathematical model for upflow packed or fluidized bed the axial dispersion and film diffusion describe the bulk phase mass transfer [5].

There are no studies in the open literature on gas dispersion/mixing study in MBR reactor having a conical bottom. The closest possible literature is for gas mixing studies in upflow packed bed [[6], [7], [8]], and expanded/fluidized bed [9], due to bed behavior of MBR from packed bed to three phase fluidized bed based on the flow conditions of the phases. All these studies used RTD concept and obtained dispersion coefficient using either moment method or modeling the test section with appropriate mass balance model having dispersion parameter. In moment method, the second moment (variance) of the RTD [10] is matched with the equation of variance for different boundary conditions [11]. In reactor modeling approach, the obtained RTD is fitted for mixing parameters of a model describing the mass flow behavior inside the test section. At macromixing level, the extreme flow conditions can be modeled using plug flow for no mixing/dispersion, and CSTR for completely mixed flow [3]. If the flow is not much deviating from the plug flow, then Axial Dispersion Model (ADM) and its many derivatives are the most common model used to describe the flow behavior [[3], [4]].

In many cases, such as in hydrotreaters, the area of interest (catalyst bed) is accompanied by additional volumes (plena). Here, by injecting tracer at the inlet and detecting at the outlet of the entire reactor will not give the required RTD information of the test section (catalyst bed). In these instances one injection and two-point measurement methods are implemented.

In one injection and two-point measurement method, is an injection-

sampling concept in which an injected tracer at the inlet of the reactor is sampled before and after the test section, and the difference in the variance of the two obtained RTD gives the effective dispersion coefficient of the test section. It is based on the assumption that the spreading of tracer or variance of the curve is linearly changing along the reactor [[11], [12])]. [6] used this approach with a step input to find the mixing of gas phase in a two-phase packed bed column.

Luhan([13]) advanced one injection and two-point detection method by integrating this injection-sampling concept with convolution and regression principle. In this approach the test section is modeled with appropriate model and the solution of the model is considered as the RTD response of the test section, the response of the test section is convoluted with the RTD signal sampled at the inlet. The convoluted signal is theoretical RTD at the outlet of the test section based on the model parameters and for the inlet boundary condition obtained by sampling at inlet of test section. The theoretical output response is regressed with actual output response obtained from sampling of tracer at the outlet of test section for minimum error to estimate mixing parameters. [13] implemented this method on a slurry bubble column reactor and [14] followed this approach on pebble bed reactor to obtain dispersion parameters of gas phase in plenum and bed zone (test section) of these reactors. They also measured the RTD curve along the radial profile at the inlet of the bed section and found similar curves radially. The significance of this radial study is that it shows the tracer from the plenum is evenly distributing to the bed section. The one injection and two-point measurement method is not applicable to the cases where the plenum are not evenly distributing the phases to the bed section. As a single point measurement at the outlet of the plena does not represent the actual flow behavior of the plena. The similar scenario is observed in MBR due to conical bottom of the catalyst bed (test section) and complex internal of plena.

The solution to this problem is an alternative injection-sampling concept called two-point/multiple injections and one detection method. In which the tracer is injected at inlet and outlet of the test section and detected at the outlet of the reactor after a mixing cup to ensure even distribution of tracer at the detection cross-sectional plane [15]. [16] used this method and compared with one injection and two-point detection method, and found both method yield similar results when experimental RTDs are interpreted with theoretical models using danckwerts boundary.

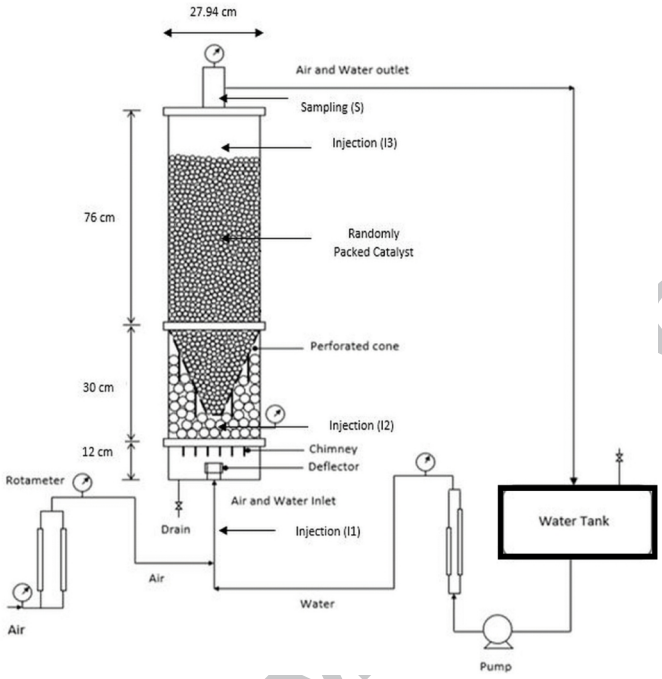


Figure 1: Schematic diagram of scaled down MBR setup for gas dynamics studies

This study focuses on investigating the gas mixing behavior at various flow condition in the catalyst bed section of MBR reactor. The approach followed is a injection-sampling concept based on multiple injection and one detection method along with convolution-regression principle approach proposed by [13]. This objective is achieved by developing a gas tracer experimental facility for MBR based on the experimental facility developed by [13] for slurry bubble column reactor and [14] for pebble bed reactor. This experimental facility has multiple injections and one sampling port and provisions to obtain the RTD curve only for gas phase from the two-phase upflow at different sections of the MBR. The RTDs of different sections along with ADM and Ideal CSTR-PFR model for packed bed and plena respectively, is used with convolution-regression to estimate dispersion/mixing parameters of catalyst bed section.

2. Experimental Setup

The experimental set-up of the moving bed hydrotreater (MBR) reactor is scaled down to pilot-plant scale from industrial scale based on hydrodynamic and geometric similarity. The scaled down flow operating condition is obtained by matching the LHSV and gas-liquid volumetric flow rate ratio with the industrial operating conditions.

Table 1: Reactor design parameters and experimental condition for gas dispersion/mixing study

Parameters	Value/Range	Comment
Column Diameter	27.94 cm	
Column Height	118 cm	
Bed Height	63 cm	Height from top of the cone to the top of the bed at no flow rate
Catalyst	3 mm Diameter	Bulk Density (570 Kg/m^3)
Liquid (Water) Superficial Velocity	0.01 to 0.4 cm/sec	
Gas (Air) Superficial Velocity	1.28 to 5.13 cm/sec	
Scaled Down Liquid Flow Rate	0.0175 cm/sec	By matching LHSV of industrial and scaled down reactor
Scaled Down Gas Flow Rate	7.7 cm/sec	By matching Gas/liquid volumetric flow rate of industrial and scaled down reactor

The schematic of the pilot plant scale reactor is shown in Figure 1. The

reactor is a plexiglass column of height 118 cm and the internal diameter of 29.7 cm. It is divided into three sections by distributor plate and conical bottom. The parts below conical bottom are called plena, and it is further divided into lower and upper plenum. The lower plenum consists of the deflector and 19 chimneys. The chimneys are attached to the distributor in triangular pitch and have an additional side hole opening just below the distributor plate (Figure 1). The upper plenum is the compartment between the conical bed and the upper plenum wall which is tightly packed with passive spheres to cover the entire region between the conical bottom and distributor plate. Above the conical bottom is bed section, which is the region from conical base to the top of the bed at cylindrical column, It is filled with 3mm industrial grade HDM (Hydrodemetallization) catalyst. The conical bottom is perforated, and perforations are small enough to avoid catalyst plugging. At industrial operation, the catalyst withdrawal is facilitated through the cone.

The ancillaries for the reactor are gas and liquid rotameters, liquid pump, and water tank. This reactor operates in upflow state, with premixed gas-liquid which is under control by rotameters are fed mixed into the deflector of the lower plenum. For scaled down operating conditions the flow profile inside the lower plenum will have a gas pocket around the chimneys side hole. The gas penetrates through the side hole, and liquid enters through main hole of chimney at its bottom both are mixed below the distributor and ejects as a spray to upper plenum. The passive spheres in the upper plenum distribute the incoming phases and are fed to the bed section through the perforated cone. The distributed stream maintains the bed in packed or expanded bed state based on the flow conditions. For scaled-down operating condition, the bed behaves as packed bed with slight expansion at the top of the bed.

In this study, the gas dispersion is investigated by varying flow rate of gas and liquid and at the scaled-down experimental condition. The dimensions of the experimental setup and operating conditions used in this study are shown in the Table 1.

3. Gas Dynamic Tracer Technique for Evaluation of the Residence Time Distribution (RTD) of the gas phase in the gas-liquid upflow MBR

The residence time distribution (RTD) concept is developed long time ago for flow evaluation of reactor by developing a model for the reactor and

quantification by RTD [[17], [11], [18]]. Its simplicity has made it an useful part of engineering applications, but simplicity lies within a particular range of applications such as single phase small-scale reactors. The complication arises when the multiphase flow is encountered; it can be difficult to separate a phase from a mixture and analyze them for tracer for RTD determination [18]. The trouble increases when reactors have plena, and the RTD is only needed for the reactor-bed section, where the conversion occurs. To overcome these difficulties, [13] developed dynamic gas tracer experimental and mathematical approach for slurry bubble column. The developed dynamic gas tracer experimental technique and a mathematical approach for a slurry bubble column reactor is used and implemented by [14] on a pebble bed reactor. Here we extend this to upflow moving bed reactor (MBR). The developed tracer technique for MBR can separate gas phase from the mixture of gas-liquid.

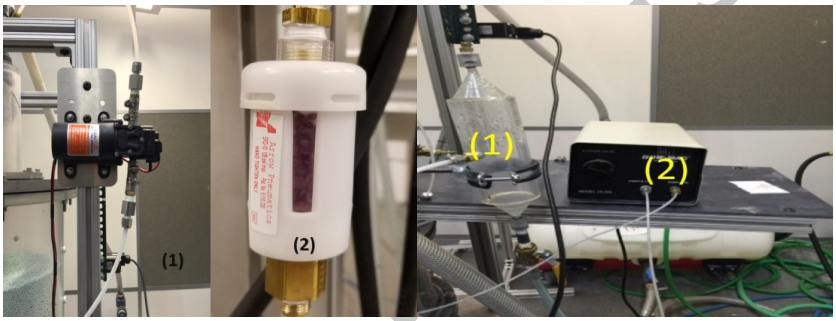
3.1. Dynamic Gas Tracer Technique

Figure 2 shows the components of the gas tracer technique. Gas tracer is analyzed using a Thermal Conductivity Detector (TCD- Gow MAC 20 series) (Figure 2a). Helium is used as a gas tracer, which is non-reactive, non-transferable to liquid phase [13], and having the physical property similar to the gas phase (air) [3]. Different kind of gas tracer are used for RTD studies based on the detection equipment and is summarized by [3]. Nitrogen (Figure 2b) is reference gas for the TCD. Water pump (Figure 2c) removes tracer laden gas-liquid mixture out of the reactor. In house developed Gas-liquid separator (Figure 2d (1)) separates gas from the liquid using a gas-pump (Figure 2d) and before gas pump there is a moisture remover (Figure 2c). These components along with data acquisition system (Gow-Mac) and reactor forms gas dynamic tracer system.

3.2. Gas Tracer System of MBR

Figure 3 shows the gas tracer system of MBR. Helium is injected through injection tubes (I1, I2, I3), detailed explanation of the injection and sampling is given in section 4.1. Compressed helium gas cylinder (Figure 2b) is connected to a solenoid valve using nylon tube (0.5 inches), and the connection continues to injection points. The solenoid valve is controlled by a digital timer and set for 0.5 sec opening interval; this provides a pulse injection. The tracer sticks to the gas phase and follows its path along with the liquid phase. The gas-liquid mixture enters into mixing cup as shown in the Figure

(a) Gas Analayzer(TCD) (b) Helium(Tracer),Nitogen(Ref)



(c) 1-Water Pump, 2-Moisture Re- (d) 1-Gas-liq Seperator, 2-Air Pump mover

Figure 2: Gas tracer components

3, and after that, sampling (S) of the mixture is done using sampling tubes and water pump (Figure 2c), which draws out the mixture and feeds into an in-house developed gas-liquid separator (Figure 2c). This pump creates a suction to remove gas phase from the separator and then it passed through a moisture remover (Figure 2c), and then only gas phase to the TCD (Figure 2a). The thermal conductivity of the helium mixed in the gas phase is compared with the reference gas (Nitrogen) for TCD. The helium mixture in gas has higher thermal conductivity than reference gas, and TCD response as voltage signal is linear with the concentration of helium in the air. Response from the TCD is amplified and recorded as time series at a sampling frequency of 10 Hz. Each injection will give respective RTD and will be used all together in developed methodology to determine gas dispersion parameter of the catalyst bed alone.

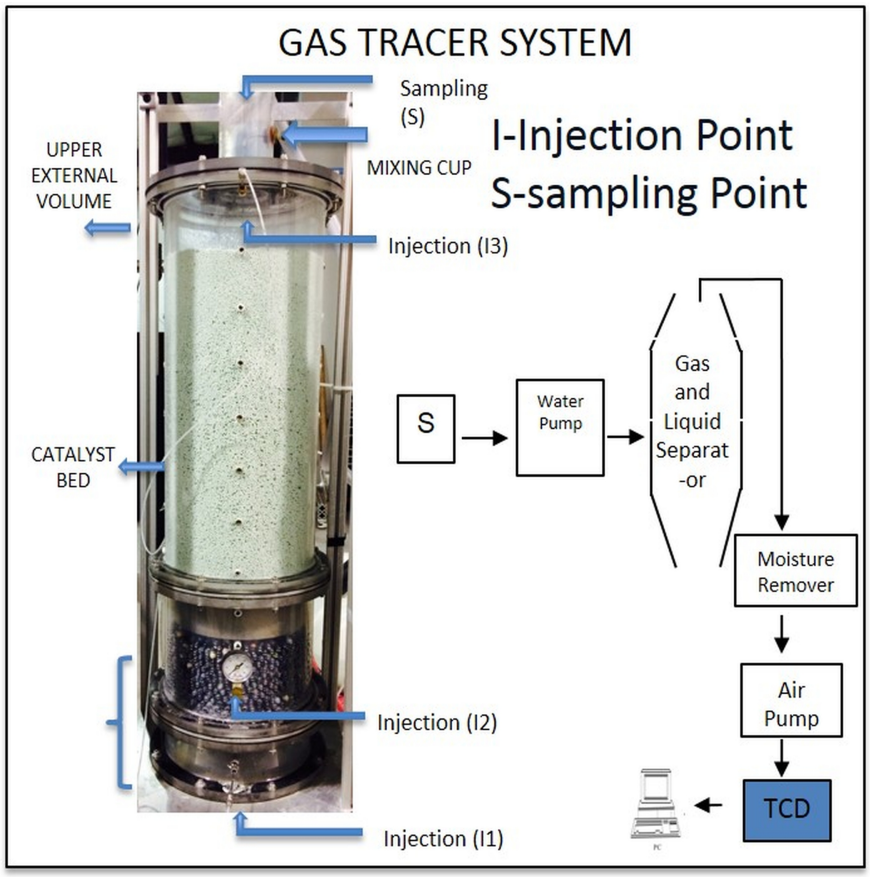


Figure 3: Gas dynamic tracer system of MBR

4. Methodology to Measure Gas Dispersion in Catalyst Bed Section of MBR

A methodology is developed based on the injection-sampling concept called multiple injection and one detection method, and a mathematical approach based on convolution and regression proposed and implemented by [13]. This particular method is developed for upflow moving bed reactor (MBR), but this method can be applied to any multiphase reactors with plena.

Table 2: Injection and sampling assembly of MBR for gas dynamics study

Measurement	Injection	Sampling	Dispersion Zones
C(1)	I1	S	**Zone(1)**: Plena + CatalystBed + Upper external Volume + Sampling Line (measurement Volume)
C(2)	I2	S	**Zone(2)**: Catalyst Bed + Upper External Volume + Sampling Line (measurement volume)
C(3)	I3	S	**Zone(3)**: Upper External Volume + Sampling Line (Measurement Volume)

4.1. Injection and Sampling Assembly

Injection-sampling assembly is designed in a way to have one point measurement (S) with three injections (I1, I2, I3) as shown in the Figure 3. Table 2 shows the zones covered by each injection and sampling point. The injection (I1) is at the bottom of the reactor and just below the plenum section, injection (I2) is below the conical bottom, and injection (I3) is just above the catalyst bed as shown in the Figure 3. The sampling (S) at the top of the reactor. The measurement C(1) (I1-S) gives RTD of the entire reactor which includes the plena, catalyst bed section, upper external volume from above the bed to sampling point, sampling assembly, and measurement system line. The measurement C(2) (I2-S) gives the RTD of zones other than plena, and measurement C(3) (I3-S) gives the RTD of the zones other than plena and catalyst bed section. The RTDs of each section are plotted in Figure 4 for industrial scale down conditions.

The shape of the RTD curve depends on the type of injection and flowing structure [3]. The injections are usually of the pulse, imperfect pulse, step, sinusoidal, ramp and parabolic in nature [3]. In the majority of the studies, mixing characteristics of phases are investigated using pulse injection [3]. In our case, we injected tracer as pulse, and if the reactor mixing behavior is between plug flow and perfectly mixed CSTR, then the response of the system for pulse injection will be of Gauss Jordan distribution type [3], as

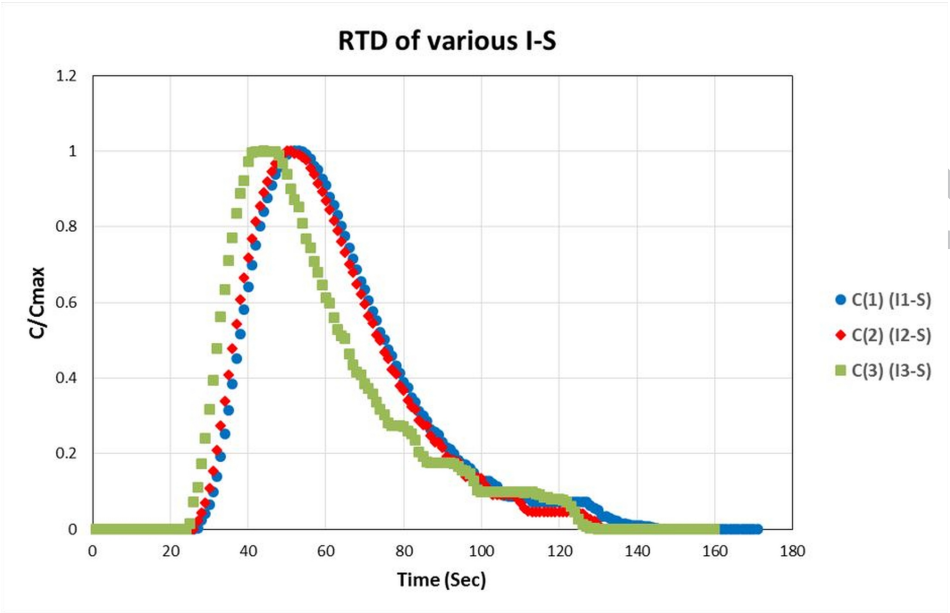


Figure 4: RTD of various injection-sampling at scaled experimental conditions

also observed from the Figure 4. We also observe step-like behavior towards the tail region for all the signals. This phenomenon is mainly due to the recirculation zones seen in the joint areas of upper external volume, which also consists of mixing cup (Figure 3). These recirculation's create pseudo-dead zones which leads to slow and late removal of tracer from these regions, and it can contribute towards the occurrence of step-like signals at the tail region. The tracer flows through the upper external volume to obtain all the signal C(1), C(2) and C(3), as seen from Table 2, and hence show step signal towards the tail regions. The RTD curves are usually plotted by normalizing it with its peak value [[19], [13], [14]] and are used to determine holdups, mass transfer parameters, and linear isotherms parameters [19], the same is done here. The plots are normalized based on the maximum concentration for each RTD signal.

4.2. Convolution and Regression Approach to Estimate Gas Dispersion in Catalyst Bed of MBR

Convolution principle is widely used to get the RTD signal of the region which is accompanied by additional volume hence additional dispersion. De-

convolution in another mathematical way to extract out the signal of the interested zone by removing dispersion for additional volumes from the overall signal, but this method is usually not preferred in chemical engineering applications due to numerical instability [13]. Convolution integral shown by equation 1 is a mathematical way to obtain RTD of a system for any arbitrary input [3]. In equation 1, C_{in} in the inlet concentration or input and C_{out} is the response of the system and C^*_{out} is the output of this system for an inlet concentration profile of C_{in}. Both input (C_{in}) and system response (C_{out}) can be obtained by proposing a model and regression to estimate model parameters, or directly from experimental RTD for a Dirac pulse input.

$$C^*_{out} = \int_0^t C_{out}(t').C_{in}(t-t').dt' \tag{1}$$

The different regions of the reactor either additional volumes or zone of interest, can be modeled by simple or complex differential type model following diffusional type mixing or stage-wise macro-mixing model where mixing is described by perfectly staged regions [4]. The complexity of the model increases with its increase in parameter, and it tries to characterize the realistic flow pattern. Some of these models are summarized in the review of [3].

The reactor shown in Figure 3 has three regions; catalyst bed section, plena (Additional volume), upper external space plus sampling line (Additional volume). ADM is the most commonly used model for the packed bed dispersion studies, here ADM is the assumed model for the catalyst bed with two parameters D_g (Dispersion coefficient) and Gas Holdup (ϵ_g). Ideal CSTR plus PFR series is the assumed model for the plena (lower plenum, packed bed region between the conical bottom and distributor plate), as CSTR is the most commonly used model for plenum for upflow reactors ([13]), and RTD experiment gives the response of upper external volume (I3-S Figure 4). Then a single point multiple injection methods (section 4.1) is implemented along with convolution and regression to get ADM parameters. ADM is solved by two-step process, In first step; by determining the concentration for inlet boundary condition for ADM, which is the solution of ideal CSTR+ PFR model (quantifies mixing in plena). In the second step; solving ADM numerically for the closed-closed boundary with inlet concentration from step 1, and parameters for regression. If the ADM or ideal CSTR plus PFR are

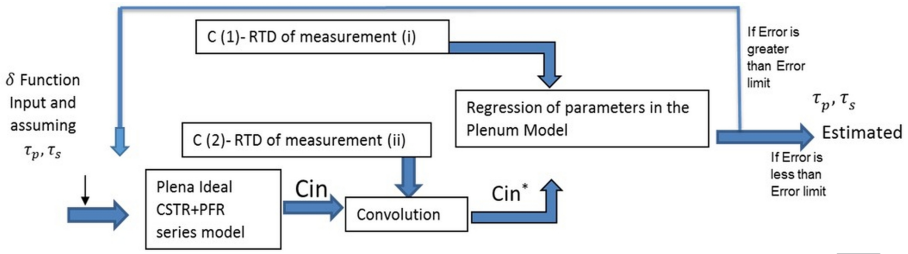


Figure 5: Schematic of convolution and regression approach to obtain parameters for plenum model

not a valid model to quantify the gas mixing process in catalyst bed section and plena, then it fails during regression test.

4.3. Step 1: Procedure to Obtain Plenum Model Parameters and Inlet Boundary Condition for ADM

Figure 5 show the schematic of the procedure of step 1. The plena are taken as ideal CSTR and PFR (equation 2), and it has two parameters τ_p (Space time of PFR) and τ_s (Space time of CSTR), the parameters are at first assumed to initiate the run for step 1. The assumed parameters give C_{in}, which is theoretically input to the section zone-2 (Table 2).

$$C_{in}(t) = 0, t < \tau_p$$

$$C_{in}(t) = \left(\frac{e^{\frac{-(t-\tau_p)}{\tau_s}}}{\tau_s}\right), t > \tau_p \tag{2}$$

Applying convolution principle; C_{in} is the input to the Zone 2 (Table 2) and the response of the Zone-2 is measured by I2-S as shown in Figure 4, C(2) is obtained experimentally by (I2-S) (Figure 4)

$$C^*_{in} = \int_0^t C_{in}(t').C(2)(t-t').dt' \tag{3}$$

The convolution gives C^*_{in} (Figure 6) which is the theoretical output of the zone 2 (Table 2), for an input concentration of C_{in} which represents mixing behavior of gas in plena, as shown in Figure 6. Hence C^*_{in} represents the theoretical RTD of the entire reactor (Zone 1) as it comprises of Plena and

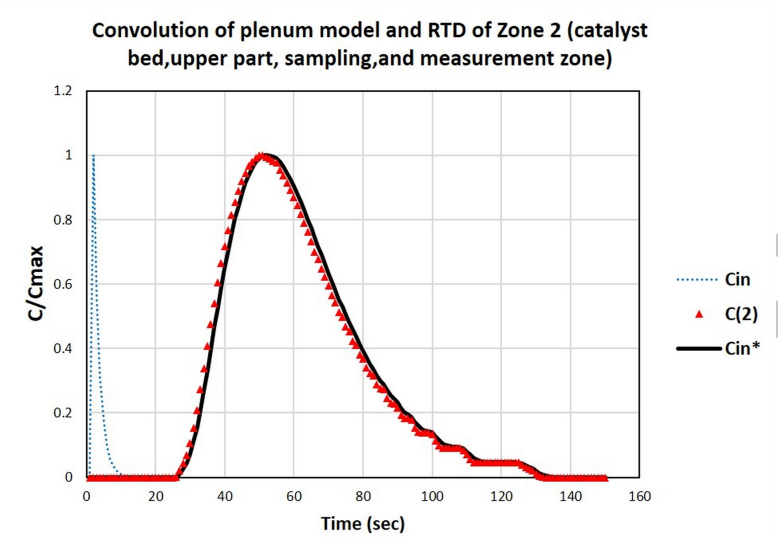


Figure 6: C_{in} (solution of plenum model; ideal CSTR+PFR), $C(2)$ (experimental response of zone-2 measured by I1-S), C^*_{in} (convoluted signal of C_{in} and $C(2)$)

Zone 2. Experimentally we have determined RTD for the whole reactor (Zone 1) $C(1)$ by I1-S. The regression of C(1) (experimental) and C^*_{in} (theoretical) for τ_p and τ_s yields these parameters for minimum error of averaged squared error in the time domain (equation 4). The n in equation 4 is the number of data points.

$$Error = \frac{1}{n}\sum_{j=1}^{n}[C^*_{in}(t_j) - C(1)(t_j)]^2 \tag{4}$$

Figure 7 shows the plot of theoretical output based on plena model and experimental output of the whole reactor for minimum error for the equation 4. The estimated regression parameter are τ_p (1sec) and τ_s (1sec) for scaled down operating conditions. The error in the equation for the estimated parameter at scaled down experimental conditions is 0.00041 and this indicates that the assumed model is valid enough to represent the gas mixing in plena. The regressed τ_p and τ_s parameter are plugged into equation 2, which is used as an initial concentration for inlet boundary condition of ADM.

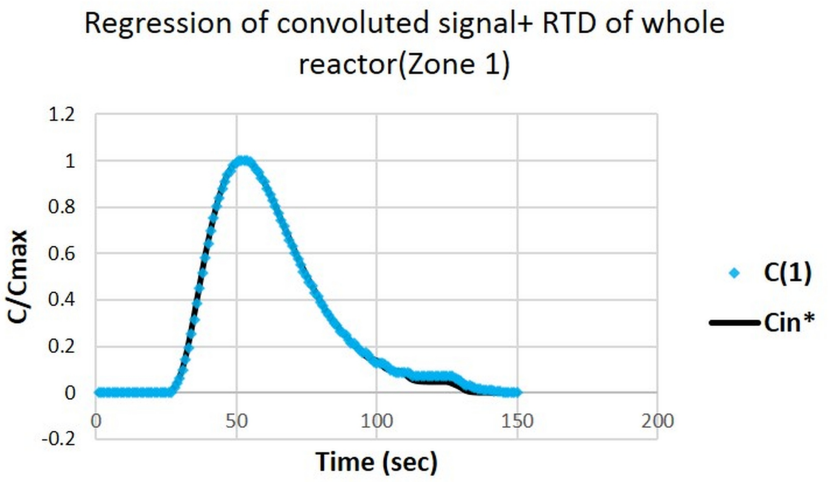


Figure 7: Regression of the theoretical output based on the plenum model (C_{in^*}) and the experimental output (C(1)) of the whole reactor for minimum error

4.4. Step 2: The Procedure to Obtain ADM Model Parameters using Step 1 Inlet Boundary Condition

The catalyst bed section shown in Figure 1 and Figure 3, is modeled using Axial dispersion model (equation 5) with boundary condition (equation 6 and 7). The parameter of ADM are D_g (gas dispersion coefficient) and ϵ_g (gas holdup). The ADM is solved numerically by plugging C_{in} in equation (6) from the C_{in} obtained from step 1 (Figure 5), and initiate the procedure (Figure 8) by assuming the parameters (D_g, and ϵ_g). The solution of ADM yields C_{out}, which is output of ADM for inlet concentration of plena as shown in Figure 9. In other words C_{out} is the theoretical RTD of plena plus catalyst bed section for dirac pulse input. C_{out} is also an theoretical input for Zone 3 (Table 2).

$$\frac{\partial C_g}{\partial t} = D_g \frac{\partial^2 C_g}{\partial Z^2} - \frac{U_g}{\epsilon_g} \frac{\partial C_g}{\partial Z} \tag{5}$$

Boundary Conditions:

$$Z = 0, U_g.C_{in} = U_g.C_g|_{z=0} - D_g \frac{\partial C_g}{\partial Z}|_{z=0} \tag{6}$$

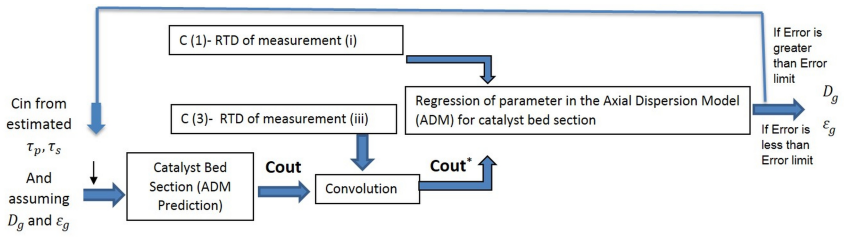


Figure 8: Schematic of convolution and regression approach to obtain parameters for ADM model using input profile C_{in}

Applying convolution principle (equation 8); C_{out} is the input to zone 3 and C(3) is experimental response of zone 3 obtained by I3-S (Figure 4).

$$Z = L, \frac{\partial C_g}{\partial z}|_{z=L} = 0 \tag{7}$$

The convoluted output C_{out^*} represents the output of the zone 3 for input profile C_{out}, (which represents the RTD of plenums plus catalyst bed section). Hence C_{out^*} represents the theoretical output of the entire reactor or zone 1. Experimental output of the zone-1 is obtained by C(1) (I1-S) (Figure 4).

The regression of C(1) (experimental) and C^*_{out}(theoretical) for D_g and ϵ_g yields these parameters for minimum error of averaged squared error in time domain (equation 9).

$$C_{out^*} = \int_0^t C_{out}(t').C_3(t-t').dt' \tag{8}$$

The two parameter regression by equation involves unconstrained regression of parameters [19]. One of the parameter (ϵ_g) is constrained between ϵ_{gmin} and ϵ_{gmax} as shown by equation 10, this improves accuracy and speed of regression calculation. Peclet number (Pe) is also estimated using equation 11.

$$Error = \frac{1}{n}\sum_{j=1}^{n}[C_{out^*}(t_j) - C(1)(t_j)]^2 \tag{9}$$

$$\epsilon_{gmin} = \frac{U * t_1}{L}, \epsilon_{gmax} = \frac{U * t_2}{L} \tag{10}$$

Whereas, U is superficial velocity of gas based on empty column, L is the

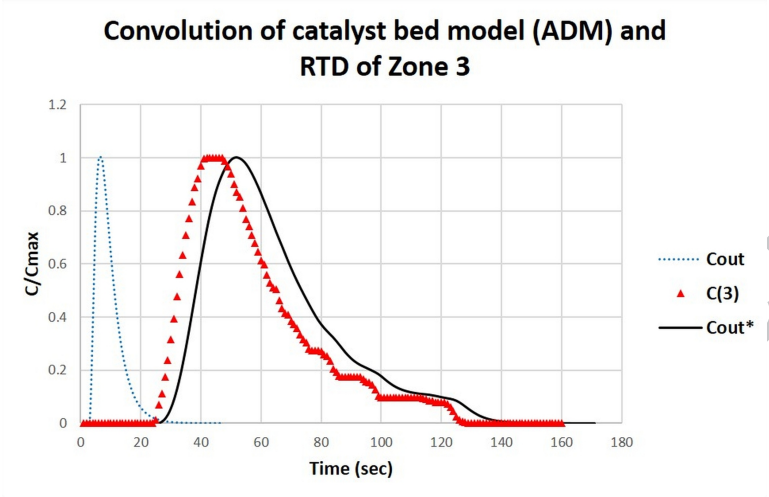


Figure 9: C_{out} (ADM solution of plenum model input), C(3) (experimental output of zone1), C_{out^*} (convoluted signal output of C_{out} and RTD of zone3)

linear distance between injection (I2 and I3), t_1 is time difference between first signal arriving for C(2) and C(3), and t_2 is the time difference between mean residence time (equation 16) for C(2) and C(3), ϵ_g is the gas holdup in packed bed, D_g is the gas dispersion coefficient.

$$Pe = \frac{U * L}{\epsilon_g * D_g} \tag{11}$$

Figure 10 shows the regression for minimum error of equation 9 for parameter D_g and ϵ_g The estimated regression parameters are D_g $(0.1m^2/s)$, ϵ_g (0.0823), and Pe (7.87) for scaled down operating conditions. The minimum error for experimental scaled down condition is 0.00051, which is lower than the tolerance limit of 0.001, and hence validates that the ADM is a valid model to represent gas dynamics in catalyst bed of MBR. This methodology is applicable for the catalyst bed section of the MBR reactor for gas dynamics investigation. In addition to these parameters, dimensionless variance (σ_D^2) is calculated for the bed section of MBR using the RTDs (Table 2) , which also indicates the degree of mixing, with σ_D^2 of zero indicates plug flow and σ_D^2 of one indicates complete mixing.

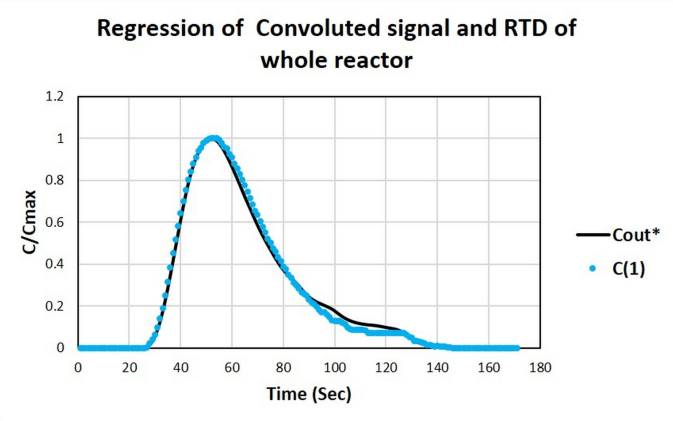


Figure 10: Regression plot of C_{out^*} (convoluted signal of ADM output and experimental output of zone-3 (I3-S)) and C(1) (experimental output of zone1) for minimum error

5. Dimensionless Variance (Tank in Series)

Tank in series is modeling concept, where n tanks are modeled as ideal CSTR in series for pulse injection of tracer. The theoretical residence time distribution (RTD) obtained from the model is regressed with experimental RTD of non-ideal reactor by varying the number of tank (n). Larger the value of n indicating the flow is towards plug flow and lower means the flow is towards CSTR. [20] showed that equation 12 is the generalized RTD for n tank modeled as ideal CSTR in series.

$$E(t) = \frac{t^n}{(n-1)!\tau_i^n} e^{-t/\tau_i} \tag{12}$$

Where τ_i is the means residence time in single tank, n is the number of tank, and τ_i is equal to τ/n, and τ is mean residence time of entire reactor. Equation 12 is converted to dimensionless form $E(\theta)$ as shown in Equation 13.

$$E(\theta) = \tau E(\theta) = \frac{n(n\theta)^{n-1}}{(n-1)!} e^{-n\theta} \tag{13}$$

Where θ is the ratio of t and τ. The variance of equation 13 can be found using equation 14, which is called dimensionless variance (σ_D^2), and this dimensionless variance is equal to the ratio of variance (σ^2) and square

of mean residence time (t_m).

$$\sigma_D^2 = \frac{\sigma^2}{{t_m}^2} = \int_0^\infty (\theta - 1)^2 E(\theta) d\theta \tag{14}$$

[20] showed the solution of equation 14 is equal to the inverse of number of tanks (n), as shown in equation 15.

$$\sigma_D^2 = \frac{\sigma^2}{{t_m}^2} = \frac{1}{n} \tag{15}$$

This indicates if σ_D^2 is zero then n is infinity, which is the case for plug flow, and when σ_D^2 is one then is n is one, which means complete mixing. Dimensionless variance can be determined by RTD experiments, as it is the ratio of variance (σ^2) (second moment) and square of mean residence time (t_m) (first moment).

$$MeanResidenceTime(t_m) = \int_0^\infty E(t) t dt \tag{16}$$

$$Variance(\sigma^2) = \int_0^\infty (t - t_m)^2 E(t) dt \tag{17}$$

In our case, the area of interest is packed bed region, and its dimensionless variance is evaluated by finding the variance of RTD of zone 2 (t_{m2}) (Figure 4 and Table 2) and RTD of zone 3 (t_{m3}) (Figure 4 and Table 2) using the equation 16 and similarly the variance (σ_2^2 and σ_3^2) using equation 17. Volume of Zone 2 minus volume of zone 3 gives volume of bed , and as these moments are additive the bed variance will be ($\sigma_2^2 - \sigma_3^2$) and mean residence time in the bed will be ($t_{m2} - t_{m3}$). Hence the σ_D for the bed is calculated using equation 18.

$$\sigma_D^2(Bed) = \frac{(\sigma_2^2 - \sigma_3^2)}{(t_{m2} - t_{m3})^2} \tag{18}$$

Equation 18 shows the dimensionless variance of the gas phase in catalyst bed region and for scaled down experimental condition (Table 1), σ_D^2 is 0.232.

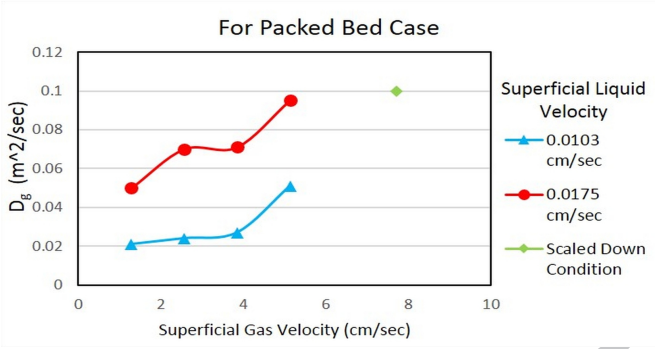
6. Results and Discussion

Gas transport inside a reactor with packing is mainly occurring due to three mechanism; bulk flow due to pressure gradients, diffusion due to concen-

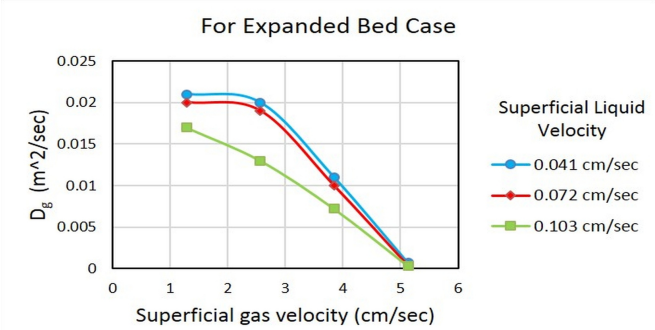
tration gradients, and convective dispersion due to spatial velocity fluctuation [21]. The summation of last two parameters defines the dispersion/mixing of phase in the system. The D_g values estimated from ADM equation is a lumped parameter indicating both molecular diffusion and convective dispersion (hydrodynamic mixing) [12] in 3-dimensional space of catalyst bed. Hence, our focus of this study is to see dispersion/mixing behavior of gas in terms of D_g values. The value of D_g functionally depends on the ratio of the particle diameter to column diameter, fluid density and viscosity, superficial velocities of phases, ratio of the length of the reactor to the column diameter, particle size distribution, and effect of temperature [8]. In this study, we wanted to see the effect of superficial velocity on the dispersion coefficient (D_g), peclet number (Pe), and dimensionless variance (${\sigma_D}^2$) in the catalyst bed section of MBR.

6.1. Effect of Flow Rate of Phases on Gas Dispersion Coefficient (D_g) for Catalyst Bed in MBR

Figure 11 shows the trend in D_g values for varying superficial velocity of the gas at low liquid superficial velocities (Figure 11a) and at high liquid superficial velocities (Figure 11b). Figure 11a shows that the Dg values are increasing with increase in gas flow rate and liquid flow rates, and this phenomenon is usually observed in packed bed reactor [[12], [8], [14]]. To understand the effect of velocity on D_g in packed bed , let us look into the equation $D_l = {D_m}' + ud/Pe_L(\infty)$ [[22], [12], [8]]. For packed bed, the estimated D_g is the summation of molecular diffusivity (${D_m}'$) and dispersion due to turbulent or eddy motion of flow i.e, convection ($ud/Pe_L(\infty)$). At low particle Reynolds number; less than 1.8 for gases, molecular diffusivity plays a vital role (Edward 1968). On increasing the velocity, the flow moves towards the turbulent flow, and eddy diffusion plays a dominant role in gas transport due to spatial velocity variations and fluctuations. The dispersive component due to eddy diffusion ($ud/Pe_L(\infty)$), depends on interstitial velocity which in turn depends on packing structure, flow distribution, and flow rates. Hence, increase in flow rate increases the convective dispersion component ($ud/Pe_L(\infty)$), and also results in the increase in bubble breakage phenomena due to the interaction of gas bubbles with catalyst bed particles ([23]). Hence, on increasing gas flow rate, we observe wider bubble size distribution which results in wider spread of gas phase along the 3-dimensional space of catalyst bed and increased mixing due to the convective component of dispersion. Both of these mechanism leads to increase in the estimated D_g



(a) Plots of D_g for varying flow rate of gas at low liquid velocity



(b) Plots of D_g for varying flow rate of gas at high liquid velocity

Figure 11: Gas dispersion plot for varying flow rate of phases

value with increase in gas flow rate. From dispersion/mixing point of view increasing the gas velocity at low liquid flow rate is good, as it increases the overall mixing, reduces channeling [12], provides better radial distribution [14]. At scaled down experimental condition, visually, the bed is behaving in packed bed state with slight expansion at the top of the bed. The results (Figure 11a) also confirm that the bed is behaving as packed for these flow rates. The gas phase flow dynamics completely change when the bed starts to expand and which we observed for the higher flow rate of the liquid.

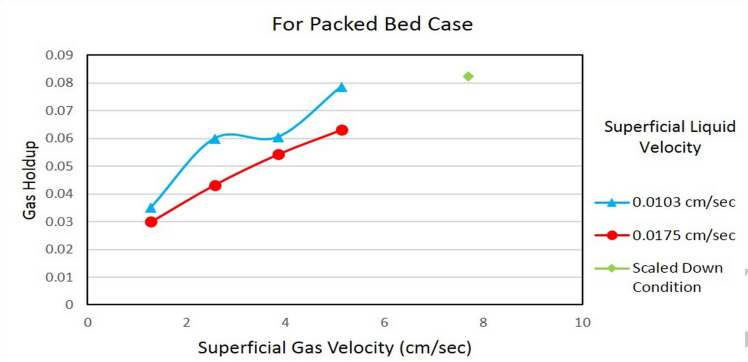
Figure 11b shows decreasing trend of D_g value with increase in both gas and liquid flow rates, which is complete opposite trend of the phenomena observed for packed bed case (Figure 11a). It shows the bed is not anymore

in packed bed state and the bed expansion is significant at the higher flow rate of liquid [19] which promotes backmixing. It is seen that with the increase in gas and liquid velocities result in more expansion of the bed and bed flow dynamics move towards the 3-phase fluidized bed. At expanded bed conditions the gas phase can displace suspended solid phase and gas phase follows least resistance path, which results in a less cross-sectional distribution of gas phase at these conditions. Although overall the bed is at high turbulent condition due to movement of solid particles, but due to less spread of gas phase along the cross-section results in the reduction in estimated values of D_g. In terms of mixing this condition is not good for hydrotreating applications. As the bubbles try to coalesce and move without dispersing cross-sectionally, which results in inefficient utilization of catalyst. Hence it is desired to run this reactor at the conditions of packed bed with least and preferably no expansion of the bed. By looking at the trend of D_g value for expanded bed, it looks the flow is more towards the plug flow state. Usually in three-phase fluidized bed the gas phase flow as plug flow with significant backmixing of the liquid phase [24]. To see how much deviation the gas flow is from plug flow, Pe and σ_D^2 evaluation is needed. To estimate Pe, ϵ_g values are needed. For three phase flow, ϵ_g is the function of flow rate and packing [25] and is one of the estimated parameter from the ADM equation 5 which is discussed in section 4.4, and its variation with flow conditions are measured to calculate Pe (Equation 11).

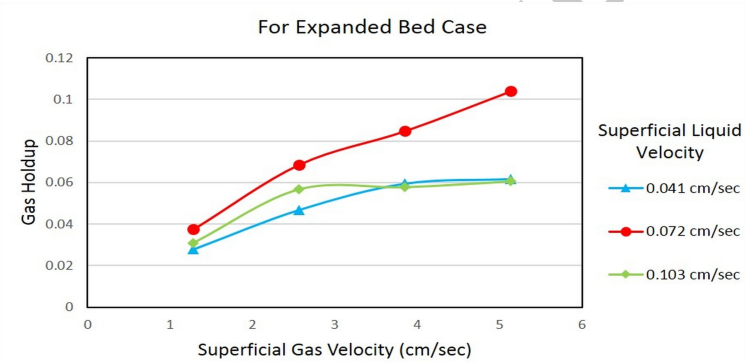
6.2. Effect of Flow Rate of Phases on the Gas Holdup (ϵ_g) in Catalyst Bed of MBR

From dispersion plot (Figure 11), we were able to identify the flow rates at which the bed behaves as packed and expanded bed, respectively. The gas holdup results are also shown for packed bed (Figure 12a) and for expanded bed (Figure 12b). Figure 12a shows that with the increase in gas flow rate there is an increase in the gas holdup and with the increase in liquid flow rate there is a decrease in the gas holdup. This behavior is expected in packed bed reactor [26], as increasing gas flow rate results in better radial distribution of gas phase [14] and thus increasing the residence time of the gas phase, and increased residence time is equivalent to increase in the gas holdup for flowing system. When the liquid flow rate is increased, the gas phase moved out quickly and reduces the residence time hence reduces the gas holdup [26].

Figure 12b shows the gas holdup at expanded bed state for varying flow rate of phases. The trend of the gas holdup is increasing with gas flow



(a) The gas holdup plot for varying gas flow rate at low liquid flow rates



(b) The gas holdup plot for varying gas flow rate at high liquid flow rate

Figure 12: Gas holdup plot for varying flow rate of phases

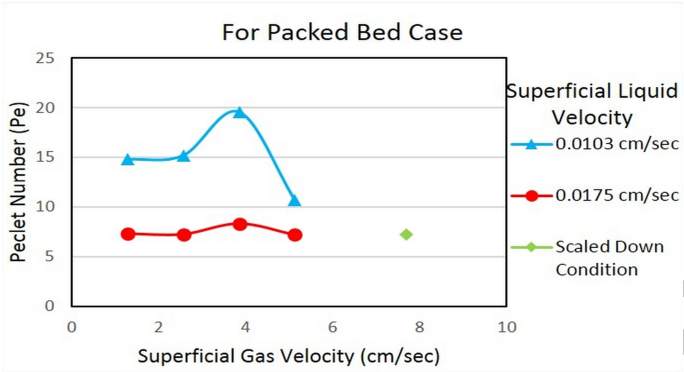
rate, similar to packed bed case. With the increase in liquid velocity, the trend is fluctuating. On increasing the liquid velocity form 0.0041 cm/sec to 0.072 cm/sec the gas holdp increases, and from increasing the liquid velocity from 0.072 cm/sec to 0.103 cm/sec the gas holdup decreases, this kind of trend is due to the degree of bed expansion. When the flow is increased from 0.0041 cm/sec to 0.072 cm/sec, the bed expands and reduces the solid concentration [27], which in turns increases the gas holdup, as much more voidage is available for gas to distribute. As the bed is in the expanded state, hence, we expected the gas holdup to increase further when the liquid velocity is increased from 0.072 cm/sec to 0.103 cm/sec, but the gas holdup

decreased, and it is due to bed behavior shifts more towards the three-phase fluidized bed. At this state the bed is expanded, thus the solids are easily displaced by moving gas phase, and on increasing the gas velocity results in bubble coalescence and movement through least resistance path, which results in increased bubble rise velocity and further reduction in gas holdup [[27], [28]].

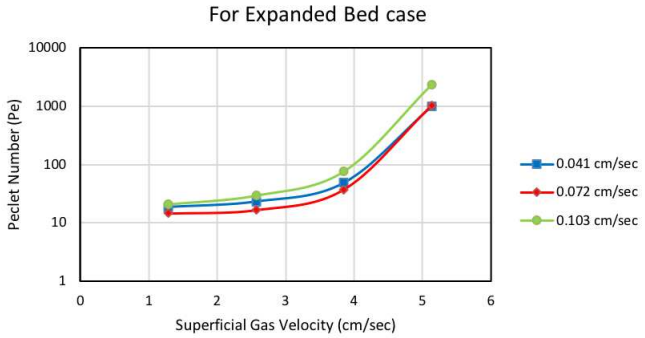
For hydrotreating purpose, gas to liquid mass transfer on the catalyst surface is the rate-limiting step, and for high utilization of catalyst, high gas holdup at high solid concentration is required, which is observed at scaled down conditions. Based on the results this is occurring at low liquid and high gas flow rate where the bed is behaving as packed bed.

6.3. Effect of Flow Rate of Phases on Peclet Number (Pe) in Catalyst Bed of MBR

Using the D_g and ϵ_g values, Pe is calculated using equation 11. Pe is a dimensionless number which gives the information of the dominance of transport mechanism between bulk flow and dispersive force. Higher the Pe means bulk flow forces dominate the transport, and lower Pe indicate the dispersion dominates flow through the bed. Figure 13a shows the trend of Pe variation for varying flow rate of gas and liquid phase, and at these flow rates, the bed behaves as a packed bed. Figure 13b shows the trend of Pe variation with the varying flow rate of gas and liquid phase at which the bed is in the expanded state. Figure 13a trends show that the Pe is not varying much with the increase in gas flow rate and decreases with increase in liquid flow rate. With the increase in gas phase the dispersive forces are increases as observed in Figure 11a, but this increase is due to the convective dispersion component of (D_g). It indicates that at these flow rates the increase in disperse force is proportional to the increase in bulk flow force and making the Pe values almost constant. With the increase in liquid flow rate, the gas dispersion is increased, as observed in Figure 11a and Pe number is also increase (Figure 13). It means at similar gas flow rate for higher liquid flow rate dispersive forces are dominating for gas transport for packed bed case, which increases overall gas dispersion/mixing in the bed. Figure 13b trend shows that with increasing gas flow rate for any liquid flow rate, the Pe increases, which means bulk forces are dominating the transport mechanism. With increases in liquid flow rate, the Pe varies but is again depended on the degree of expansion. Overall as the bed moves towards 3 phase fluidized bed the Pe increases which means reduced dispersion/mixing of gas phase or



(a) Peclet Number plot for varying flow rate of gas at low liquid flow rate



(b) Peclet Number plot for varying flow rate of gas at high liquid flow rate

Figure 13: Peclet number plot for varying flow rate of phases

moving towards plug flow.The results indicate that gas dispersion/mixing is better at packed state for higher liquid flow rate and at the higher gas flow rate. The scaled down conditions (Figure 13a) in terms of mixing is good, as it comes under the purview of packed bed with slight expansion at the top. At these flow rate, the gas mixing is good, but overall gas distribution is largely function of plena and bed packing. To confirm the findings from the results of D_g and Pe. A dimensionless variance (σ_D^2) is calculated for the bed section, which also indicates the dispersion/mixing behavior of phases.

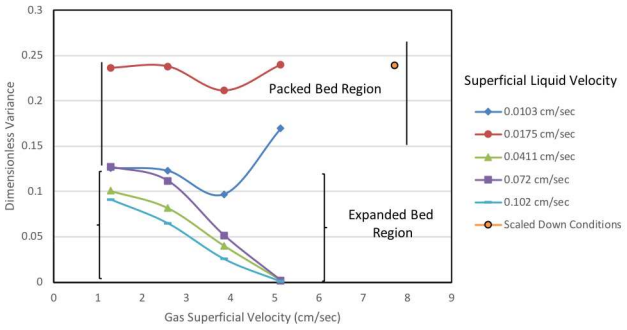


Figure 14: Dimensionless variance of gas phase in the catalyst bed for various flow conditions and scaled down conditions

6.4. Effect of Flow Rate of Phases on Dimensionless Number ($\sigma_D{}^2$) in Catalyst Bed of MBR

The dimensionless variance for the catalyst bed section is calculated from the RTDs using it moments (t_m, σ^2), as explained in the section 4.1. If its values is zero then it means the gas movement is in plug flow manner, and if its one then the flow is completely mixed. Figure 14 shows the dimensionless variance in the catalyst bed for various flow condition and at scaled down conditions and it also indicates packed/expanded bed operating condition. Overall for all the flow condition the values are close to zero, indicating the gas flow is closer to plug flow. As for σ_D^2 less than 0.1 is usually considered to be in plug flow of packed bed reactor [29]. Relatively, gas dispersion/mixing is more in packed bed region, and in this region increasing liquid velocity and gas velocity increases dispersion/mixing, and in the expanded bed region the flow is moving closer to plug with increase of both gas and liquid velocities. The results are similar to what we observed from the results of Dispersion (Figure 11) and Peclet number (Figure 13). The gas dispersion/mixing is higher in the packed bed region and even for scaled down condition compared to the expanded bed regions.

7. Remarks

Gas dispersion/mixing has been investigated for the catalyst bed section of the pilot-scale upflow moving bed hydrotreater reactor (MBR), using injection-sampling concept based on multiple injection and detection method,

and a mathematical approach of convolution and regression, with appropriate model for catalyst bed and plena proposed by [13]. The catalyst bed is Modeled with Axial Dispersion Model (ADM), with its inlet boundary condition obtained from the Ideal CSTR plus PFR model of plena, these models are assumed first and validated based on the regression. This methodology is successfully implemented in the MBR at the scaled-down experimental condition and various other flow rates of phases.The dispersion plot indicates that at low liquid flow rates the D_g increases with increases in gas flow rate and decreases with increase in liquid flow rate, this trend is observed in packed bed state. At higher liquid flow rates the D_g is decreasing with increase in both gas and liquid flow rate, and this trend is observed in expanded bed state. Pe plot shows that the in packed bed state the flow is relatively dominated by the dispersive forces and in expanded bed state gas flow moves towards plug flow state with the increase in bed expansion. This is confirmed by calculating ${\sigma_D}^2$, which indicate overall the gas phase flow is towards plug flow, but at expanded bed state the flow is more closer to plug flow. Hence, a good gas mixing is achieved for highest flow condition of phases where the bed expansion is minimum, and that is seen in the scaled-down experimental condition.

8. Acknowledgments

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Highlights

- Estimation of Gas Mixing/Dispersion Parameter (D_g, Pe, σ_D^2) for catalyst bed
- At low liquid flow rate, the bed is in packed bed and it expands for increasing flow
- Gas mixing/dispersion is higher in packed bed state
- For all flow conditions, the gas flow is not deviating much from plug flow
- Scaled down flow condition is good in terms of mixing and catalyst utilization