CFD Simulation of Raschig Ring Packing Patterns in a Pilot Scale: Prediction of Mean Residence time

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Abstract

Mean Residence Time (MRT) was determined numerically for the pilot packed bed reactor filled with the ceramic raschig rings. Three well-defined patterns and one randomly packed bed were studied, where a tube-toparticle ratio (N) was around 7. A case study of Dry Methane Reforming (DMR) was investigated at 600 °C, 1 atm. Reactant feeding rates were varied in the range of 0.985 to 2.957 L/min. The MRTs of four difference packing pattern, namely, vertical-staggered (pattern 1), chessboard-staggered (pattern 2), reciprocal-staggered (pattern 3), and randomly packed bed were conducted using finite-element based Computational Fluid Dynamics (CFD). The results were shown in terms of E(t) function where a higher value of the E(t) function means greater deviation from the ideal plug flow. Results showed that chessboard-staggered pattern had the lowest E(t) values compared with all patterns and all feeding rates. To deeply representative results for the system configurations, the discussion on nonideal behaviors of each structured packing can be made systematically in this work.

Keywords : Mean Residence Time, Residence Time Distribution, Packed Bed Reactor, Dry Methane Reforming and Computational Fluid Dynamics

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1. Introduction

Residence Time Distribution (RTD) has been fundamentally exploited to characterize the flow behaviors of reactors in the areas of petrochemical and chemical processes. The RTD can be estimated directly to precise the required MRT in order to obtain a desired reaction yield. It is useful not only for sizing reactors, but also for troubleshooting existing reactors. Gas phase through a microstructured falling film reactor, the RTD was studied to develop an appropriate flow model for mass - transfer characteristics in the gas phase of the system [1]. A theoretical approach to RTD analysis was also used for Tubular Fixed - Bed Reactor (FBR), multi slit Integrated Micro Packed Bed Reactor - Heat Exchanger (IMPBRHE) [2], rectangular channel herringbone structures [3], and gas-liquid micro-fixed beds [4]. The approximation of RTD method can be applied to the more complex geometry. Packed bed reactors are generally filled with a small object such as pellets or a complex structure such as raschig ring, porous ring, or balls depending on specifically designed structured packing. Sebastian Zuercher [5] has studied the ceramic foams bed structure in catalytic gas cleaning process using the dispersion model to quantified back mixing. A good design should have a good momentum distribution with an acceptable pressure drop to save pumping costs. In addition, controlling the desired pressure drop and uniform velocity distribution over the bed increases the diffusion efficiency of the reactants.

Besides the RTDs parameter, mean residence time (MRT) is a significant consideration indicating whether a certain process or reaction can be carried out to the desired degree of completion [6]. The MRT is the average time particle spends in the investigated system before it reaches a designed point along its flow path [7]. For mini-channel reactor, the two-phase flows were investigated in terms of MRT and RTD. The results showed that liquid phase had much longer of RTD and MRT than gas phase. Estimation of the unidirectional dispersion indicated it was the combined effect of evaporation and condensation inside the minichannel which affected the MRT and RTD. Unlike the fixed bed, the dispersion resulted from the doubledirection diffusions [8]. From the above mentioned, the RTD were obtained by using the tracer experiment studies which are injecting an inert tracer at the inlet and measuring its concentration at the outlet of the reactor.

Computational approaches have come to be seen as effective tools to investigate non-ideal behaviors of flow systems in term of RTD analysis [6]. However, computational estimation of MRT for a non-ideal heterogeneous catalytic reactor has not yet been proposed. Especially in a gas-solid system containing distinct hydrodynamic patterns due to various catalytic packing structures. Therefore, this work differs from the previous one in that it highlights coupling the RTD with the raschig ring packing patterns in pilot packed bed reactors. The main goal of this study is to measure both the effects of packing patterns and the RTD deviations from the ideal plug flow regime. By application of the CFD technique, the behavior of complex systems influenced by a large number of flow, fluid and geometric parameters can be predicted. The methodology was used for testing on a catalytic packing system of dry methane reforming. Modeling and simulation were carried out by finite-element analysis using the software COMSOL based MULTIPHYSICSTM 3.5. Flow patterns (in 3-D) of reactant gases in a packed bed were expected as the solutions in which fluid velocity and pressure profiles can be displayed. According to availability of velocity gradients, a post processing equation to estimate MRT was proposed. The MRT for each corresponding structured packing and various gas flows was calculated and compared with that obtained from ideal plug flow correlation.

2. Methodology and Simulation Model

In this work CFD was used as a computational technique in verifying MRT of a reactor filled with solid catalyst pellets in three structured packing and one randomly packed bed. The COMSOL MULTIPHYSICSTM 3.5 program was selected as an effective tool to simultaneously solve the governing equations relying on the conservation principles of mass and momentum. Simulation results gave insight into the physics behind certain packing patterns. The ceramic raschig ring catalyst was a single channel with an inside diameter of 0.55 cm, an outside diameter of 1.2 cm, and the pellet was 1.29 cm long. The raschig ring was packed in the reactor size 10.16 cm in diameter and 5.16 cm long. Two stainless plates were installed on both sides to create a set of realization of close-packed packing. In order to explore the impact of structured packing of the rasching ring catalyst in the reactor, three practical structured packing and one randomly structured packing were selected as shown in Fig. 1.

2.1 Governing Equations and Mathematical Models

Hydrodynamics of gaseous flow was explained by simultaneously solving the Navier-Stokes equations, i.e., nonlinear momentum and continuity equations:

$$\rho \frac{\partial u}{\partial t} - \nabla . \eta \left(\nabla u + \left(\nabla u \right)^T \right) + \rho u . \nabla u + \nabla p = F \qquad (1)$$

$$\nabla_{.u} = 0 \tag{2}$$



Fig. 1. Computational domain of catalytic structured packing of the raschig ring within the packed bed reactor. a) Vertical Staggered, b) Chessboard Staggered, c) Reciprocal Staggered, d) Random Packing

- Where, η is the viscosity of fluids [kg/(m s)]
 - u is the velocity vector (m/s)
 - ρ is the density of the fluid (kg/m³)
 - p is the pressure (atm)
 - F is a body force term
 - n is a normal vector

The boundary condition is shown in Table 1.

Table 1 Boundary conditions

Boundary condition	Equation		
Inlet	$u.n = u_0$		
Outflow boundary	$\mathbf{p} = \mathbf{p}_0$		
No slip (reactor wall and stainless	u = 0		
plates)			
Slip symmetry condition (catalyst	u.n = 0		
surfaces)			

2.2. Mean Residence Time (MRT)

To visualize the computational approach proposed for the determination of MRT of a packed bed reactor, Dry Methane Reforming (DMR) at 1 bar and 600°C was chosen as a modeled case study. Here reactant gases consisting of methane (CH₄) and carbon dioxide (CO₂) were converted to synthesis gas products, i.e. carbon monoxide (CO) and hydrogen (H₂) (Eq. 3). To avoid coke formation as a possible side reaction, very precise residence time of a few seconds was needed to be controlled for a tubular plug flow operation.

Dry Reforming Reaction;

$$CH_4 + CO_2 \longrightarrow 2CO + 2H_2$$
 (3)

In this work, four different arrangements of pellets; vertical staggered with 32 pellets, chessboard staggered with 32 pellets, reciprocal staggered with 30 pellets, random 28 pellets were considered. The void volumes (V) of each structured packing configuration were 3.39×10^{-5} m³, 3.39×10^{-5} m³ 3.62×10^{-5} m³ and 3.21×10^{-5} m³, respectively. For all packing patterns,

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reactant feed rates (\dot{v}) was also investigated in the range of 0.985 - 2.957 L/min. The constructed geometries are depicted in Table 2. As the reactor volume and feed rate have been specified, therefore, mean residence times, τ can be obtained from the design equation of an ideal plug flow reactor assuming no volume change due to reaction as illustrated in Table 2.

$$\tau = \frac{V}{\dot{v}} \tag{4}$$

Where; V is the void volume of the reactor, which obtaining from $V = V_{reactor} - V_{bed}$.

 \dot{v} is the volumetric flow rate of the fluid and

au is the MRT of the fluid of an ideal plug-

flow.

A conventional way to estimate the MRT in a chemical reactor is to analyze the RTD from tracer experiments. Normally, the quantity E(t) is obtained as a function of the residence time distribution (RTD). It is the function that describes in a quantitative manner how much time different fluid elements have spent in the reactor. The exit concentration of a tracer species C(t) can be used to define E(t) as illustrated in Fig. 2 and Eqs. (5) - (7).

$$E(t) = \frac{C(t)}{\int_{0}^{\infty} C(t)dt}$$
(5)

Such that:
$$\int_{0}^{\infty} E(t) dt = 1$$
 (6)

The MRT or $\mathbf{\bar{t}}$ of the reactor can be calculated from integral forms as in Eq. (5).



Fig. 2. a) Plug flow model b) packed bed model and E(t) diagram.

Instead of having RTD data from tracer experiments to describe the flow regimes within plug flow reactors, a more convenient way to investigate laminar flow behaviors in such systems was proposed in this work. A computational approach using CFD technique was exploited to solve for normal velocity profiles of reactant gases within a packed bed reactor.

A generalized form of Eq. (8) was introduced using parameters \overline{z} as mean residence distance of a system. The mean residence distance stands for an average distance that fluid elements will travel along a packed บทความวิจัย

volume. The \overline{Z} term includes an effect of structured packing via integration of local velocity response (u_i).

$$\overline{Z} \cong \frac{\sum_{i} Z_{i} u_{i} \Delta Z_{i}}{\sum_{i} u_{i} \Delta Z_{i}}$$
(8)

As a first step, hydrodynamics of all packed bed patterns was analyzed. For validating the simulation results, post-processing needed to be done by integration of the boundary velocity correlations. To estimate the net flow through the axial direction Z, the mean residence distance \overline{Z} represents a parameter that combined the influences of the flow field in terms of distribution velocity (u_i) and distance (Z_i) of the main flow. Obtaining the mean residence distance, the net flow can be done by drawing a graph between the velocity distributions in the axial plane with the main flow. This data can be collected through the results of flow models. However, in order to obtain a graph of the velocity and distance, the data, i.e. normal velocity (u_i) and distance of fluid from the inlet (Z_i) needed to be collected. The domain was divided into groups of planes, which were not continuously recorded. To find an average velocity of each plane, domain areas of the image plane were defined at a height showed in Fig. 3a. According to a catalyst layer, each layer has a height equal to 1.29 cm for the catalyst pellets situated in a vertical direction and height of 1.201 cm for

catalyst pellets situated in the horizontal direction. Each layer was divided into a number of planes, where at the height plane was 10 relatives to the catalyst was represented by Z^{L} and the vertical height relative to the catalyst in the horizontal direction was represented by Z^{D} . After the mean residence distance \overline{Z} was calculated, the MRT can be calculated from the intensity data according to:

$$MRT = \bar{t} = \frac{\bar{z}}{u} [s]$$
(9)

$$E(t) = \delta(\bar{t} - \tau) \tag{10}$$

Where; u is the velocity of fluid (m/s)



Fig. 3. Catalyst domains and normal velocity as simulation results.

To obtain the information concerning how far that a real packed bed reactor behaves differently from an ideal plug flow one, the E(t) term can be formulated from the MRT obtained by a finite - element based method (\bar{t}) and an ideal plug flow correlation (τ) [5,9] as shown in Eq. (10). The values of E(t) for each structured packing and various gaseous flow rates were calculated and used for discussion on the behaviors of particular structured packing in the next section.

3. Results and Discussions

3.1 Local Flow Structures

Since the MRT depends on the actual path taken by the gas phase (reactants inside the reactor) during the journey within the raschig bed. The degree of deviation from the axial flow of an individual gas stream causes the computationally-determined MRT to differ from that obtained from plug flow basis. The changes of direction or flow splitting or detouring are forced by the packing but still under the governing laws of mass and momentum. In the following subsections, the local flow fields and the interactions between gaseous and packing phase will be investigated prior to determining the values of the corresponding MRT [6, 9-13].

3.1.1 Local Flow Structures of Vertical Staggered Packing

For the vertical staggered packing, the total number of 32 pellets was used to create the four-stories packing, which the centers of each pellet offset with the centers of the pellets of the following row (story), as shown in the insert of Table 1. Practically, the operating volumetric flow rate fell into the laminar flow regime usually adopted in this type of packed-bed reactor, namely, 0.986, 0.1577, 0.1971, 0.2366 and 0.2957 L/min. In general, as shown in the figures of Fig. 4a, the flow velocity was high at the center line of the hole of raschig ring and the accelerated flow region occurred due to the confined space between the external surface of the raschig ring and the inner wall of the flow channel. The flow direction was mainly in the axial direction. However, the flow was retarded to the stagnation point at the bottom surface of the next row raschig rings. Afterwards, in order to ensure a mass balance, the fluid stream was divided and remerged with another half of the flow stream from the neighbour raschig ring. Nevertheless, the average flow velocity was the same for each row.

3.1.2 Local Flow Structures of Chessboard-Staggered Packing

The chessboard-staggered pattern exhibited the high flow through the hole of vertical raschig rings, and a very small flow velocity within the horizontal rings. This pattern of flow distribution persisted onto the next rows.



Fig. 4. The velocity distribution of (a) Vertical-Staggered (b) Chessboard-Staggered (c) Reciprocal-Staggered.

Fig. 4b showed the sequence of flow distributions. For this packing pattern, the horizontally-align raschig rings occupied more spatial volume and caused the smaller flow area. The higher flow velocity resulted from the reduction of the flow area due to packing, and the revealed maximum velocity was higher than in the vertical-staggered packing. A finite fraction of gaseous phase must spend a long time within the packing, i.e., flowing slowly through the horizontal holes of certain rings. In addition, its flow direction changed significantly from the axial flow; however, somehow the accelerated flow restrained this effect and the resultant MRT for the chessboard-staggered packing was close to that of the vertical-staggered packing as will be shown in section 3.3.

3.1.3 Local Flow Structures of Reciprocal-Staggered Packing

From the inserts of Fig. 4c, the flow structure observed within the first row of the reciprocalstaggered packing was qualitatively the same as that of the vertical-staggered packing at each flow rate. In the second row, however, most of the gas volume flow was in the central holes of the horizontal raschig rings. The flow velocity was low in those regions except in the interspaces between neighboring rings. These reciprocal variations of flow distributions continued to the next two rows, i.e., the third and the fourth rows had a similar flow distribution to the first and second rows, respectively.

Since the high flow velocity observed from the odd rows of this packing pattern was still lower as compared to that observed in the vertical-staggered and chessboard-staggered patterns and the larger fraction of flow was in the slow flow region, it was suspected that the reciprocal-staggered packing might give the highest mean residence time. In addition, the MRT obtained from the simulation might differ vastly from that calculated using the plug flow approach.

3.1.4 Local Flow Structures of Randomly Packed Bed

Randomly-packed catalyst bed is often applied in an industrial catalytic reactor because of the ease of loading, however the characteristics of non-uniform velocity, temperature, and concentration could easily be found [14-15]. In order to extend the studies toward a conventional way of packed beds, some random packing was also investigated in this work. The total number of 28 pellets was filled into randomly packed bed reactor models, as shown in Table 2.

D 1: D //	Number	Void volume (m ³)	Flow rate		τ (sec)	
Packing Pattern	of catalyst pellets	vola volume (m)	L/min		(Eq.4)	
Vertical Staggered	32	3.39 x 10 ⁻⁵	\dot{v}_1	0.986	$\boldsymbol{\tau}_{_{1}}$	2.07
			\dot{v}_2	1.577	$\tau_{_2}$	1.29
			\dot{v}_3	1.971	$\tau_{_3}$	1.03
			\dot{v}_4	2.365	$\tau_{_4}$	0.86
			\dot{v}_5	2.957	τ_{5}	0.69
Chessboard Staggered	32	3.39 x 10 ⁻⁵	\dot{v}_1	0.986	$\boldsymbol{\tau}_{1}$	2.07
			\dot{v}_2	1.577	$\tau_{_2}$	1.29
			\dot{v}_3	1.971	$\tau_{_3}$	1.03
			\dot{v}_4	2.365	$\tau_{_4}$	0.86
			\dot{v}_5	2.957	τ_{5}	0.69
Reciprocal Staggered	30	3.62 x 10 ⁻⁵	\dot{v}_1	0.986	$\boldsymbol{\tau}_{_{1}}$	2.21
			\dot{v}_2	1.577	$\boldsymbol{\tau}_{_2}$	1.38
			\dot{v}_3	1.971	$\tau_{_3}$	1.11
			\dot{v}_4	2.365	$\tau_{_4}$	0.92
			<i>v</i> ₅	2.957	τ_{5}	0.74
Randomly Packed Bed	28	3.21 x 10 ⁻⁵	\dot{v}_1 \dot{v}_2	0.986	$\boldsymbol{\tau}_{_1}$	3.09
			\dot{v}_2	1.577	$\tau_{_2}$	1.93
			\dot{v}_3	1.971	$\tau_{_3}$	1.54
			<i>v</i> ₄	2.365	$\tau_{_4}$	1.29
			\dot{v}_5	2.957	τ_{5}	1.03

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To compare with the well-defined patterns, the studied volumetric flow rate fell into the similar laminar flow regime, namely 0.986, 1.577, 1.971, 2.365 and 2.957 L/min. From the simulation results of the random packing, the local flow velocity in each row of these packed was found not uniform and had its characters due to the positions of approaching rings. In order to explain the results of the randomly packed beds showed in Fig. 5, local flow velocity distribution inside and around each ring was impacted by two factors; which were the ring's position itself and the positions of its surrounding rings. At the first row, the ring's position itself played an important role in the local velocity distribution. The two definite positions, i.e. vertical and horizontal raschig rings can be systematically explained. In the case of vertical raschig rings, the gases would rather flow through the middle hole of the raschig ring and the void volume between the rings. The vertical rings clearly promoted the axial flows in the middle hole and the radial flow direction only at the upper and lower annular surface, and thus some local turbulence around the entrance and exit of the middle hole can be found. For the raschig rings in horizontal position, the gases dispersed all over the outer surface of these rings, and a very slow flow was found in the middle holes. As some of the raschig rings in the randomly packed models were in the positions between vertical and horizontal placement, so that the local velocity distribution was observed as a combination of the vertical and horizontal flow

behaviors depending upon the angle of its place. This is reasonable due to the fact that the fluid would prefer to go through the path with minimum resistance, and channeling flow was typically developed. In the opposite way, some parts within the randomly-packed beds faced with the situation which was lacking of fluid flows or stagnant zones. The channeling and stagnant behaviors found in the randomly packed beds could result in the uneven distribution of fluid flows within the reactor, and that definitely affects to the MRT of the reaction system.



Fig. 5. Total velocity and velocity vector in the Random Packing.

3.2 Effect of Packing Pattern on the Mean Residence Time

To optimize the mean residence time, it is especially important to consider the packing pattern in packed bed reactors. For the pilot scale, how packing pattern affects the mean residence time is an important consideration in order to obtain a uniform and well defined flow through the packed catalyst. The effects of channeling, recirculating and stagnant zone are problems for packed beds using complicated packing

from the finite element method, i.e. 1.0-3.2 sec, were

packing method. Atmakidis (2009) studied the residence time distribution in different spherical packing methods. For the residence time distribution, two compared methods are investigated. The first method is the tracer method and the second is the post processing method. Results found a channeling effect in near wall and zero velocity areas. Two methods gave similar results on the residence time distribution [16]. Therefore, in order to investigate the effect of packing pattern, the research aimed to investigate the MRT which was calculated from the finite-element based method and calculated from the ideal plug flow basis and were shown in Fig. 6. For the verticalstaggered packing (Fig. 6a), the mean residence times obtained from the finite element method, i.e. 0.8 - 2.4 sec were higher than that obtained from the plug flow calculation, i.e. 0.6 - 2.0 sec at all flow rate 0.985-2.957 L/min respectively. The averaged difference of the mean residence times obtained from both methods is about 20% difference. Similar behavior and trends of the mean residence times can be observed for the chessboard-staggered shown in Fig. 6b. The mean residence times obtained from the finite element method, i.e. 0.7-2.3 sec was also higher than that obtained from the plug flow calculation, i.e. 0.6-2.0 sec at all flow rate 0.985-2.957 L/min respectively. The averaged difference of the mean residence times obtained from both methods is about 13% difference. For the last packing pattern, the reciprocal-staggered pattern (Fig. 6c), the mean residence times obtained

geometries which depended on the design of size and

still higher than that obtained from the plug flow calculation, i.e. 0.7-2.2 sec, at all flow rate 0.985-2.957 L/min respectively. As seen from the Fig. 6c, somehow this pattern exhibited larger differences of the mean residence times calculated from each method approximately of 54% difference. The reason behind these differences lay in the distinct flow structures as explained in the Section 3.1.3. The flow structure observed within the first row of the reciprocalstaggered packing was qualitatively the same as that of the vertical-staggered packing at each flow rate. In the second row, however, most of the gas volume flow was in the central holes of the horizontal raschig rings. The flow velocity was low in those regions except the interspaces between neighboring rings. It was interesting that the mean residence times determined from the plug flow correlation for all three packing patterns were close i.e. vertical-staggered, chessboardstaggered, and reciprocal-staggered packing as 0.6-2.0 sec, 0.6-2.0 sec, and 0.7-2.2 sec respectively. This can be explained by seeing that the Eq. (4) was used to calculate the residence times with almost the same void fraction where the total numbers of raschig rings of 32, 32, and 30 were applied to vertical-staggered, chessboard-staggered, and reciprocal-staggered packing respectively. In the cases of randomly packed bed, the mean residence times obtained from the finite element method were higher than that obtained from the plug flow case for all flow rates. The average difference of the mean residence times obtained from both methods is about 47%. From the results, this can be explained from the flow behavior of the randomly packed beds which have no pattern. Channeling effects can appear in this kind of packed bed reactor and induce uncontrollable flow regime. Therefore, the use of mean residence times obtained from the plug flow correlation might lead to a large error in the design. It is noteworthy to mention that the finite element method using computational technique can be used to systematically identify the MRT for packing bed reactors, which can represent the values closer to that of the real reactors. This can lead us to better design in both sizing and operation of this equipment.

3.3 The E(t) function

Prior to the present study, the E(t) or delta function obtained by the integration method of the velocity correlations, as described in Section 2.2, was shown in the Fig. 7 of the flow channels with four difference structured packing in the range of feeding rate of 0.985 to 2.957 L/min.

For all pattern packing, a similar trend of delta functions and feeding rate was observed. The highest values of the E(t) have been found at the lowest values of the studied flow rates. As the feeding rate of 0.985 to 2.957 L/min, the E(t) of chessboard-staggered, vertical-staggered, and reciprocal-staggered patterns are 0.0041 - 0.0122 sec, 0.0109 - 0.0439 sec, and 0.0750 - 0.2262 sec respectively. For the randomly packed beds, the E(t) functions are in the range of 0.1353 - 0.3934 sec. The highest MRT was observed in the reciprocal-staggered packing, which can be explained that the reciprocal-staggered packing may be occurred recirculation eddy effect compared with other patterns.



Fig. 6. The mean residence times obtained from the finite-element based method (t) and the ideal plug flow correlation (τ).

On the other hand, the chessboard-staggered showed the lowest value, which tells us that this packing pattern can provide a nearly perfect distribution compared with other packing patterns. The delta function, decreased as the feeding flow rate increased in accordance with the counteraction between the effects of accelerated and slow flow regions discussed in Section 3.1. This can be explained by referring to the high shear force of fluid at high flow rate mainly induced the flow regime through an axial direction. Stagnant zone and recirculation eddies were found less at higher flow rate. Therefore, the MRTs obtained from the plug flow correlation are not far different from the MRTs obtained from the finite element method. It is also significant to point out that the MRT for packed bed reactors when operated with high flow can be reasonably estimated from the ideal plug flow correlation. This is confirmed by the relations between flow rate and E(t) function as seen by Eq. (10).



Fig. 7. The E(t) functions for each packing pattern at different feed flow rate.

4. Conclusions

The interaction between the reactant gasses and the packing of heterogeneous raschig ring flow behavior were presented in this research. Both the velocity and the MRT were different among the four packing patterns discussed herein. The highest MRT was observed in the randomly packed bed. The flow channeling and the slow flow regions that occurred locally within each packed bed emphasize the importance of the packing pattern on reactor design. The results were shown in terms of E(t) function where a higher value of the E(t) function means greater deviation from the ideal plug flow. Results showed that chessboard-staggered pattern had the lowest E(t)values compared with all patterns and all feeding rates. Thus, a careful selection of packing pattern such as in a catalytic bed reactor is so crucial. The different hydrodynamics within the bed will play a significant role in various aspects of heterogeneous reactor design. Thus, the simulation results obtained by the present research may be taken into consideration when designing this type of reactor in order to achieve the optimum conditions. The MRT and flow behavior presented here have established that the CFD simulations may be used to provide flow information that can serve as the basis for developing more complete packed bed reactor models.

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