

## FLUID DYNAMIC STUDY USING RTD IN A PACKED REACTOR AND EVALUATING FLOW PATTERN MODELS ON THE CHEMICAL CONVERSION. AN APPROACH TO REAL BEHAVIOR

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**Abstract:** In this work was done a fluid dynamic study in an experimental packed reactor using RTD exposing bimodal and modal behavior when it was varied the particle diameter and bed presenting flow channels, dead zones in the vessel and lateness of the material mixture in the equipment. Additionally, using flow pattern models was estimated the chemical conversion with greater approximation to the experimental value. This result could be use in the scaling stages of the process and minimize overdesigns.

**Keywords:** RTD, flow pattern models, packed reactor, chemical conversion

### 1. INTRODUCTION

Knowledge of the use and function of studies in catalytic reaction engineering (CRE) on the sustainable development of new technologies is importance to understand its role in the industrial processes from the transformation of the raw material to its finished product where the efficiency and profitability of the chemical reaction carried out in a catalytic reactor depends to a great extent on the right design of the catalyst, selection and design of the reactor and certain operating conditions, all of them according to the scaling of the process [1, 2].

The balance of mass, heat, and momentum provided from the knowledge and relationship between chemical kinetics and fluid dynamics allow the use of CRE as a basis for multi-stage process design [1, 3].

For chemical engineering, a right reactor design is fundamental, and generally, is ideally treated: mixed and plug flow patterns. Unfortunately, it has been observed behavior very different than expected in the real processes for which the elements contained in the residence time distribution (RTD) methodology could be used with special attention, the residence time distribution curves ( $E(t)$ ), and their cumulative ( $F(t)$ ) [4-6]. The aggregation mode of the fluid, the time of occurrence of mixing of the fluid (earliness or lateness), and the RTD behavior inside of the reactor are non-idealities considerations in the design that could be a good practice for scaling processes [4] providing information about channeling and dead zones in the reactor.

Worldwide, packed reactors are usually used with high frequency in industrial processes of basic manufacture, intermediate, and finished chemical products. Pressure drop, RTD, mass and heat transfer are crucial for the optimal design and operation of packed reactors and, therefore, the accurate estimation of these parameters is very important [7].

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The modern concept of residence time theory emerged recently from the same works from Danckwerts reintroduced the axial dispersion model. The initial assumptions are: 1. The flow pattern is in a steady state, 2. There is only one inlet and one outlet, 3. The inlet and outlet are closed, so they flow through of equipment, and 4. The concept of residence time applies to conservative entities.

The design, performance, and optimization of chemical reactors could be carried out through the characterization of the mixing phenomenon in conjunction with the chemical conversion of the reaction using as a tool the RTD analysis in the dynamics of the behavior of the fluid in the reactor [7]. This will allow for predicting the behavior of the flow in contact with the catalytic bed and provide the possibility of solving operational problems in the reactor [8-10].

For a reliable modeling, scaling, and design, it is important to describe the flow pattern. For this, a reliable approach is the use of the RTD methodology directly in the overall reactor [11, 12].

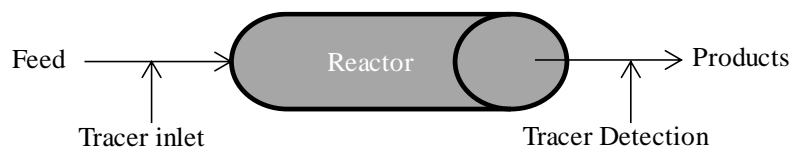


Fig. 1. Tracer in the chemical reactor.

According to de Sousa [4], the experimental determination of RTD requires a tracer that does not react, resembles the reagents, and can be detectable. Due it, to this study was used the shape selectivity theory was where the knowledge of the topology of the pores, interaction of reactants and catalytic activity is key for the molecules flow through the porous medium [13]. The behavior of the tracer should reflect the material flowing through the reactor, see Figure 1.

This work has focused to present a fluid dynamic study in a packed reactor using RTD exposing mainly the presence of flow channels, dead zones in the vessel and lateness of the material mixture in the equipment when it is varied the particle diameter and bed length. Also, an evaluation of the flow pattern models on the chemical conversion will be shown with the intention to indicate the use of models most adequate to estimate the chemical conversion in the scaling process allowing an approach to real physicochemical behavior of the process.

## 2. EXPERIMENTAL SETUP

The mathematical models and the methodology to estimate the residence time distribution, mean residence time, variance, Peclet number, are exposed by [8, 14-19] summarizing the most relevant equations as follows:

The RTD curve indicates the time of fluid particles in the reactor and it is calculated by:

$$E(t) = \frac{C(t)}{\int C(t)dt} \quad (1)$$

where  $C(t)$  is the tracer concentration at any time.

The mean residence time ( $t_m$ ) is calculated by:

$$t_m = \int_0^{\infty} t \cdot E(t)dt \quad (2)$$

The variance squared ( $\sigma^2$ ) is calculated by:

$$\sigma^2 = \int_0^{\infty} (t - t_m)^2 \cdot E(t)dt \quad (3)$$

The cumulative RTD is calculated by:

$$F_{(t)} = \int_0^t E_{(t)} dt \quad (4)$$

The reactor Peclet number (Pe) is calculated by:

$$Pe = \frac{uL}{D} \quad (5)$$

where,  $u$  is flow velocity,  $L$  is reactor length, and  $D$  is dispersion coefficient.

The dispersion is calculated using the variance method by:

$$\frac{\sigma^2}{t_m^2} = \frac{2}{Pe} - \frac{2}{Pe^2} \cdot (1 - Pe^{-Pe}) \quad (6)$$

The Damkoler number is a fundamental parameter in chemical conversion due to allowing the relationship between the chemical kinetic and the diffusion of the involved molecules [20]. The calculation for reactor Damkoler number is calculated by the equation:

$$Da = \frac{kL^2}{D} \quad (7)$$

For a first order reaction, where  $k$  is the rate constant and the determination of the chemical conversion by dispersion models and tanks in series is assuming a completely segregated fluid.

The calculation for the chemical conversion ( $X$ ) in according to [9] is by:

$$X = 1 - \frac{4q^{Pe/2}}{(1-q)^2 \exp(\frac{Peq}{2}) - (1-q)^2 \exp(-\frac{Peq}{2})} \quad (8)$$

where:

$$q = \sqrt{1 - \frac{4Da}{Pe}} \quad (9)$$

### 3. RESULTS AND DISCUSSION

A packed catalytic reactor is presented as a case study, with data set corresponding to six different experimental tests under equal pressure and temperature conditions for pentenes cracking reaction to obtain light olefins (ethylene and propylene). All of them belong to the catalytic process kinetic regime in a bench scale reactor of 25cc capacity. The experimental data are reaction temperature (500 °C), feed rate (1cc/min), the run time (0.5 to 6 h), space velocity (3 to 12 h<sup>-1</sup>), catalyst load (5 to 20 cc), catalyst particle diameter (0.6 and 1.2mm) and mass balance for each test [21].

The catalyst used in the experimental test was pentasil zeolite with a pore diameter of 0.56 nm which grants selective cracking of pentenes (molecular size 0.54nm). The feed contains cyclopentane with the molecular size of around 0.54 nm which will have the same trajectory through the pores as the pentenes without reacting in the active sites due to its chemical stability and lower reactivity with respect to pentenes which allows put forward it as a tracer in this system.

Table 1 shows the summary of the calculations involved to study the chemical conversion in a packed reactor using flow pattern models. The analysis of the results comes from the graphical interpretation of the distribution curves, for this reason, Figures 2 and 3 are presented at different lengths of the catalytic bed at two particle diameters.

For Figures 2a, 3a, 3b and 3c, the behavior of the distribution function suggest a modal shape with tail analysis indicating late micromixing in the reactor with greater pronouncement in test 1.

An explanation for this observation could be attributable to the fact that in packing with large particle diameters, the fluid tends to prefer the easiest paths in its trajectory, moving through the interparticle free spaces, while in packing for smaller particle diameters, there is less interparticle free space, providing resistance to flow and achieving its entry into the catalyst pores.

Table 1. Parameters to determine the distribution of residence times.

Test	Mean residence time, $t_m$ (h)	Variance, $\sigma^2$ (h <sup>2</sup> )	Peclet number, Pe (adim)	Damkoler number, Da (adim)
1	3.0	3.26	2.80	4.70
2	3.3	5.96	2.10	3.50
3	3.3	6.03	2.10	3.50
4	3.0	3.30	2.80	4.70
5	3.0	3.30	2.80	4.70
6	3.0	3.30	2.80	4.70

For Figures 2b and 2c the curve is bimodal indicating the possibility of channeling and dead zones in the reactor (less bed with large particle diameter leads to more interparticle free space and between the bed and the vessel inlet and outlet).

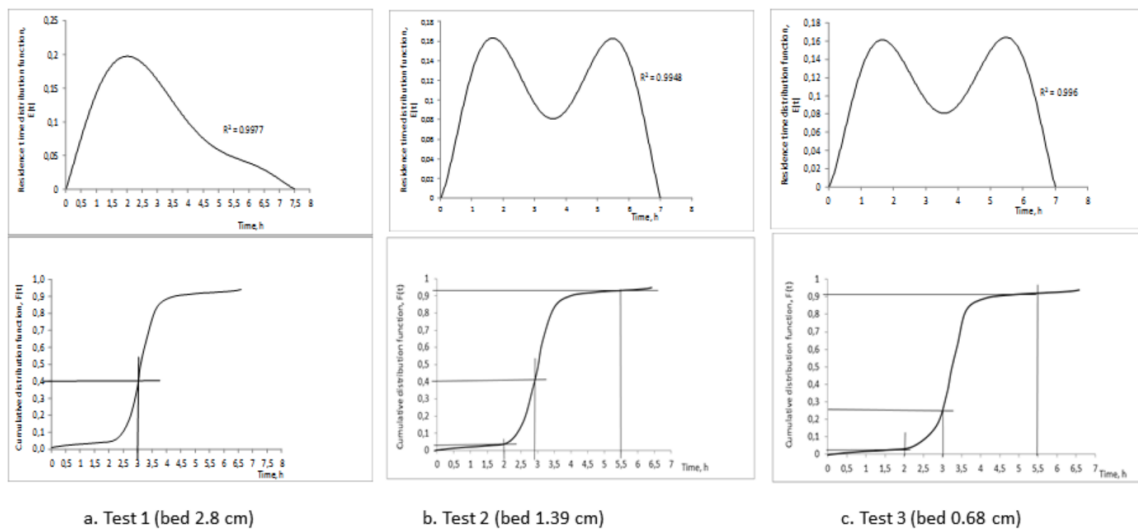


Fig. 2. RTD curve and cumulative at different bed lengths with particle diameter 1.2 mm.

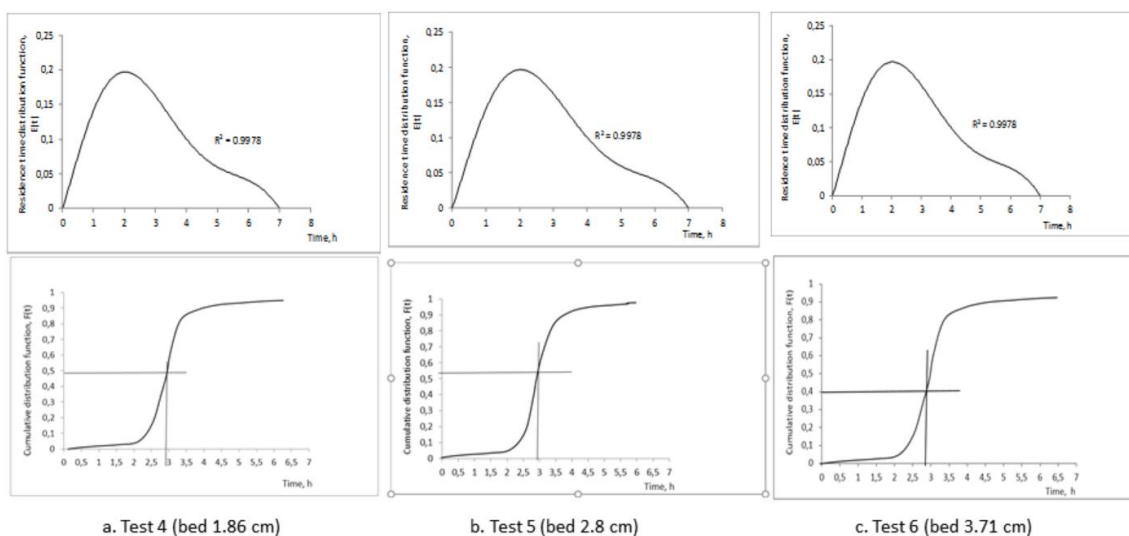


Fig. 3. RTD curve and cumulative at different bed lengths with particle diameter 0.6 mm.

The determined mean residence time trough of the cumulative distribution curve analysis was 3 h for all tests. For this time in tests 1, 2, 3 and 6 a feed fraction greater than 60% still remains inside the reactor, while for tests 4 and 5 this is 50%. The analysis leads us to think that the reaction should have more time to achieve its stabilization. The experimental stabilization time was 6 hours taking force from the aforementioned analysis. The feed fraction that remains inside the reactor could induce unwanted side reactions such as coking, shortening the life of the catalyst and the probability of generating hot spots on the walls of the reactor.

Using the information from the RTD method analysis, it was possible to estimate the chemical conversion using the flow pattern models of dispersion and tanks in series for non-ideal process, and it allowed evaluating them in comparison with the value calculated from ideal plug flow model and the real value reported experimentally. The summary of these values is shown in Table 2.

Table 2. Chemical conversion using flow pattern models.

Tests	Bed length (cm)	Particle diameter (mm)	Chemical Conversion			
			Experimental	Models		
				Piston Flow	Dispersion	Tanks in series
1	2.8	1.2	76	63	93	91
2	1.39	1.2	94	50	88	85
3	0.68	1.2	62	27	87	85
4	1.86	0.6	90	50	93	91
5	2.8	0.6	89	63	93	91
6	3.71	0.6	96	73	93	91

The primary intention of using a mathematical model is its closeness to the experimental value, to this extent, a comparative graph has been made between the estimated results of the chemical conversion using the plug flow, dispersion and tank models in series shown in Figure 4 where the percentage relative deviation is also presented. It can be seen in Figure 4 that the estimation of the chemical conversion using flow pattern models that involve hydrodynamic parameters ( $Pe$  and  $Da$ ) in the packed reactor leads to an approach toward its experimental value.

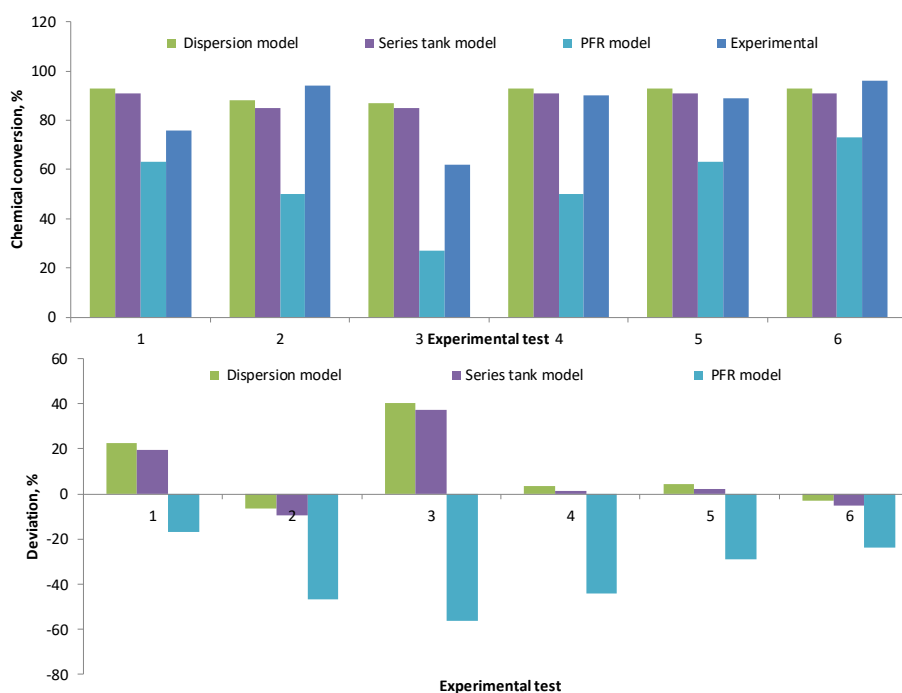


Fig. 4. Chemical conversion using different flow pattern models.

It is attributed to considering the rates of transport by convection, dispersion, and reaction that are involved in the same process during the trajectory of the fluid in the reactor. This will allow having knowledge of fluid dynamics related to chemical conversion present in the reactor to give explanations to the experimental results and an

approach to real behavior from the flow pattern models with the intention of using it in the scaling stages of the process and to be able to minimize overdesigns.

#### 4. CONCLUSIONS

The calculated Peclet number for the RTD curves with modal behavior ( $Pe = 2.8$ ) is greater than that calculated for the RTD curves with bimodal behavior ( $Pe = 2.1$ ).

In this study case, a bimodal behavior in RTD curve was obtained with a short bed and large particle diameter while modal behavior was obtained with a long bed and large particle diameter and whatever bed height with small particle diameter.

The calculated Dankholler number for the RTD curves with modal behavior ( $Da = 4.7$ ) is higher than calculated for the RTD curves with bimodal behavior ( $Da = 3.5$ ) due to changes in flow dispersion.

Using the information of the average residence times could be estimated the stabilization time of reaction in the performance regime of the process.

The dispersion of the fluid, interpreted by the calculated squared variance, is greater in a system that presents channels and dead zones (bimodal RTD curve) compared to systems with modal behavior in its RTD curve up to 85% deviation.

The retention of fluid in the packed bed is lower when the channels and dead zones (bimodal RTD curve) are present, around 50%, while the retention is up to 60% with modal behavior in RTD curves.

In a packed bed with small diameter particles (0.6 mm), micromixing is not affected by varying the length of the bed. On another hand, micromixing is affected when there is a large particle diameter (1.2 mm) and the length of the bed is varied, high lengths there is a dominant late micromixing and at low lengths, the flow dynamics of the system change due to the presence of channels and dead zones.

Flow pattern models referring to fluid dynamics (dispersion, tanks in series) in packed reactors allow estimating the chemical conversion with greater approximation to the experimental value compared to ideal models (plug flow).

The piston flow model to calculate the chemical conversion presented deviations between 17% and 56% with respect to the experimental values.

The dispersion and tanks in series models showed low deviation values (3% and 5%) with respect to experimental values, except when there is a small bed height with a large particle diameter (40%).

The best estimate of chemical conversion was achieved using the dispersion method under a system with a high bed length and small particle diameter in a packed reactor (3%).

Knowledge of fluid dynamics in packed reactors allows estimating similarity parameters for process scaling up with less uncertainty.

In future works, an estimation of the fluid dynamic parameters in a packed reactor will be carried out using specialized programs in computational fluid dynamics (CFD) to analyze the flow pattern models. As well as diverse studies in different catalytic systems.

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