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RESEARCH ARTICLE OPEN ACCESS

NON-IDEAL FLOW MODEL FOR A TUBULAR REACTOR AND A STIRRED TANK REACTOR IN-SERIES, USING STIMULUS-RESPONSE TECHNIQUES

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ABSTRACT

This work presents an experimental study on a laboratory scale about the hydrodynamic behavior of fluid flow in a tubular reactor and a stirred tank reactor in-series and varying their arrangement. The experiments were carried out using stimulus-response techniques with a tracer solution of sodium chloride in unit pulse form. The experimental results allowed obtaining the Residence Time Distribution curves R_θ vs θ for different reactor arrangements. The results obtained are similar to those reported by Levenspiel for a battery in-series with a plug flow reactor and a perfectly stirred reactor. The difference found with the studied system is that these show dead water in both equipment. The arrangement of the reactors does not modify the graph of Residence Times Distribution obtained, similar to the ideal situation presented in the literature consulted. As a result of the experimental study and the adjustment of the data, a non-ideal flow model was obtained for different kinds of reactors with dead water, connected in-series and with different arrangements. The simulation of the system for different degrees of back mixing in the system reflects a behavior similar to that of series of reactors of this type, but with ideal behavior.

I. INTRODUCTION

An important role in the analysis of any studied process is the obtention and application of models that, from the mathematical point of view, describe the physical and chemical phenomena present in the system. Many models have been used to characterize the dispersion of fluids in flow systems. The most widely used methods of handling mixing have been based on models using diffusion equations with modified diffusion coefficients. These are called dispersion models and the coefficients are called dispersion coefficients. Some explain the transverse, longitudinal dispersion or both [1-2].

The processes simulation with the help of mathematical models constitutes a scientific method of vital importance for the development of the Chemical Industry [3-10]. Within this branch, chemical reactors occupy a preponderant place, since their particular characteristics (shape, size, etc.) are related to the results of the different chemical reactions that occur within them [11-12].

This work focused on the laboratory-scale assembly of a stirred tank reactor system (RTA) and a tubular one (RT) with the aim of studying, using stimulus-response techniques, the hydrodynamic behavior in them, both individually and in-series combinations. The mathematical model that describes the hydrodynamic behavior of the indicated equipment and its series batteries, arranged in different ways, was another of the objectives of this work.

II. MATERIALS AND METHODS

II.1 STIMULUS-RESPONSE TECHNIQUES

The use of stimulus-response techniques for obtaining flow models has great application in the Chemical Industry [13-16]. With the help of these techniques, studies are carried out on the flow of fluids in various chemical equipment, allowing a better understanding about the characteristics of the equipment and therefore an optimal use of its technological possibilities.

II.2 EXPERIMENTAL SETUP

The system used was set up on a laboratory scale. For this, a glass tubular reactor 81 cm long, 1.6 cm internal diameter and a volume of 162.7 cm^3 was used; in addition, a mechanically stirred tank reactor 13.7 cm high, 10 cm internal diameter and an operating capacity of 827.2 cm^3. The inlet flow to the reactors was set with an OMEGA® model FL50001A flowmeter.

The study of the behavior of the fluid as it passes through the system was carried out using stimulus-response techniques, using 30% (w/v) NaCl as a tracer. The fluid used was water and the dose or injection portion of the tracer was 5 cm^3 as a unit impulse, measuring the concentration of the tracer over time at the end of the reactor system, for which an AZ® model AZ8306 conductivity meter was used. In this way, the solution conductivity values were obtained as it passed through the cell over time (the tracer concentration and the fluid conductivity are directly and linearly related).

The first experimental setup was carried out in such a way that the fluid that passes through the rotameter (A), enters the stirred tank reactor (B) and subsequently passes into the tubular reactor (C) where the conductivity meter (D) measures the concentration of the tracer (Figure 1).

Subsequently, the position of the reactors was inverted, that is, the fluid was first passed through the RT and then through the RTA. Also, experiments were performed on the RT and RTA individually.

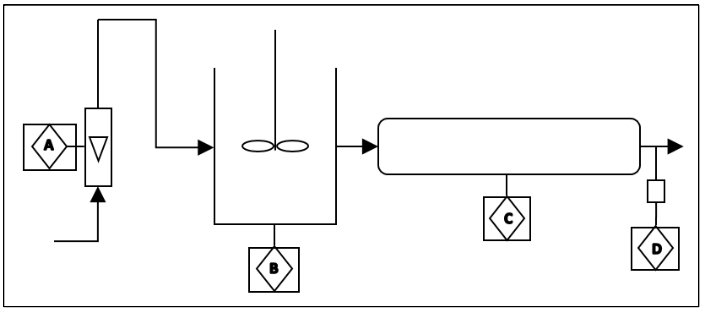

Figure 1: Laboratory-scale assembly of the stirred tank and tubular reactor system connected in series for stimulus-response studies with a 30% NaCl tracer.
Source: Authors, (2020).

We worked with a constant volumetric flow of 6.7 mL/s and in the case of the RTA it was operated with a stirring speed of 1050 rpm.

The conductivity values over time for each combination were tabulated in Microsoft Excel, then the calculations were performed according to the equations reported in the consulted literature[13] that allow us to obtain the values of C_θ vs θ (Residence Times Distribution or RTD).

II.3 DEAD WATER FRACTION CALCULATION

The dead water fraction (f_{Vdi}) in each experiment was found from the RTDs obtained in each experimental system. This fraction is proportional to the quotient between the total unit area (A_{Total}) and the area under the curve (A_i), for values of θ > 2. These calculations were performed for each reactor separately and for their series arrangements. Thus:

$$f_{V_{d1}} = \frac{V_{d1}}{V_{RT}} \propto \frac{A_{RT|\theta>2}}{A_{Total}} \tag{1}$$

$$f_{V_{d2}} = \frac{V_{d2}}{V_{RTA}} \propto \frac{A_{RTA|\theta>2}}{A_{Total}} \tag{2}$$

$$f_{V_{d(1-2)}} = \frac{V_{d1}+V_{d2}}{V_{(RT+RTA)}} \propto \frac{A_{RT-RTA|\theta>2}}{A_{Total}} \tag{3}$$

$$f_{V_{d(2-1)}} = \frac{V_{d2}+V_{d1}}{V_{(RTA+RT)}} \propto \frac{A_{RTA-RT|\theta>2}}{A_{Total}} \tag{4}$$

V_{d1} and V_{d2} are the dead water volumes in the RT and RTA, respectively; $V_{RT}=V_p+V_{d1}$ and $V_{RTA}=V_m+V_{d1}$; V_p and V_m are the volumes of a plug flow reactor and perfect mixing reactor. A_{RT} and A_{RTA} are the areas under the curve obtained from the RT and RTA system, respectively, and their serial arrangements.

II.4 MATLAB® SIMULATION

With the mathematical model obtained, which describes the experimental RTDs, simulations were performed in MATLAB® to validate the effectiveness of the model based on the dispersion number.

A stand-alone MATLAB® version 7.1.0.246 (R14) application was used. This application is suitable for computers running Microsoft® Windows XP, and is for non-commercial research purposes only.

III. RESULTS AND DISCUSSIONS

III.1 FLOW DEFECTS

A preliminary analysis of the experimental curves showed the existence of dead water in the studied systems (**Erro! Fonte de referência não encontrada. - Erro! Fonte de referência não encontrada.**). All curves show an asymptotic behavior to the horizontal axis for values of θ > 2, observing that in the stirred tank reactor this phenomenon is more pronounced. No other flow defects were observed.

III.2 MATHEMATICAL TREATMENT OF DATA

The C_θ values were normalized for subsequent analysis, being $R_\theta=C_\theta/C_{\theta máx}$ then plotting R_θ *vs* θ, which allowed obtaining the residence time curves, fitted to a following mathematical model type:

$$R_\theta = a(\theta-d)^b e^{c(\theta-d)} \tag{5}$$

Then the physical sense of the equation constants (5) was analyzed. According to Levenspiel [13] for discrete values the mean distribution time is given by:

$$\bar{t} \cong \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i} \tag{6}$$

And its variance or «*(how long)² does the curve take to pass through the measurement point*», is defined as:

$$\sigma^2 = \frac{\sum t_i^2 C_i \Delta t_i}{\sum C_i \Delta t_i} - \bar{t}^2 \tag{7}$$

Thus, defining the dimensionless variance:

$$\sigma_\theta{}^2 = \frac{\sigma^2}{\bar{t}^2} \quad (8)$$

Therefore, the constants of the proposed model (5) can be related according to the dispersion number (D/uL) [1, 2, 17].

The boundary conditions under which the system was treated respond to the «open-open» scenario where the flow is not disturbed as it passes its limits [14]: tracer injection and conductivity meter cell, respectively. For these operating conditions, the dispersion number can be calculated from the following equation:

$$\sigma_\theta{}^2 = 2\left(\frac{D}{uL}\right) + 8\left(\frac{D}{uL}\right)^2 \quad (9)$$

With the values obtained from equation (9) for each test carried out, the model constants were defined as a function of the dispersion number, so:

$$a = \frac{1}{3.7702\left(\frac{D}{uL}\right)^{1.5304}} \quad (10)$$

$$b = 2.6429e^{-8.293\left(\frac{D}{uL}\right)} \quad (11)$$

$$c = \frac{1}{\frac{2}{3}\sqrt{\sigma_\theta{}^2}} \quad (12)$$

$$d = \theta_0|_{C_\theta \neq 0} \quad (13)$$

Finally, substituting the constants in equation (5), the non-ideal flow model was obtained:

$$R_\theta = \frac{(\theta - d)^{2.6429e^{-8.293\left(\frac{D}{uL}\right)}}}{3.7702\left(\frac{D}{uL}\right)^{1.5304}} e^{\left[-\frac{(\theta-d)}{\frac{2}{3}\sqrt{\sigma_\theta{}^2}}\right]} \quad (14)$$

III.3 MATHEMATIC MODEL ANALYSIS

The mathematical model obtained (5), to which all the RTD curves of the experiments carried out fit, both individual (**Erro! Fonte de referência não encontrada.** and **Erro! Fonte de referência não encontrada.**), as their possible combinations RT-RTA and RTA-RT (**Erro! Fonte de referência não encontrada.**), is unique.

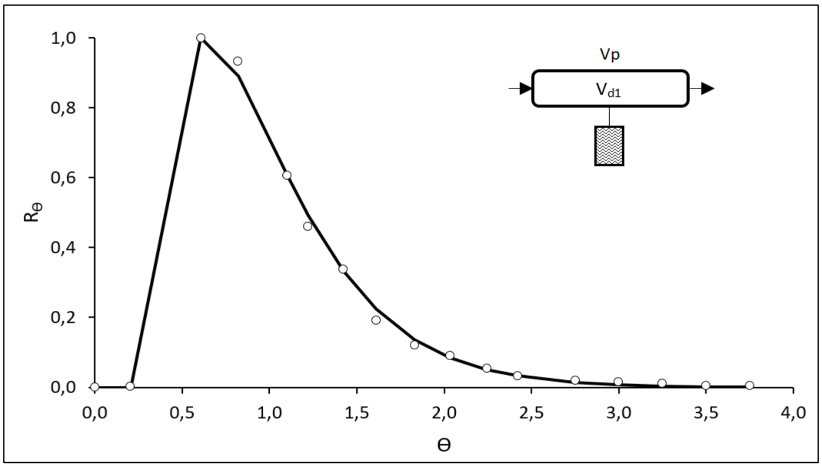

Figure 2: RTD curve for the tubular reactor with $R^2 = 0.99$, being (o) the experimental data and (-) the proposed model.
Source: Authors, (2020).

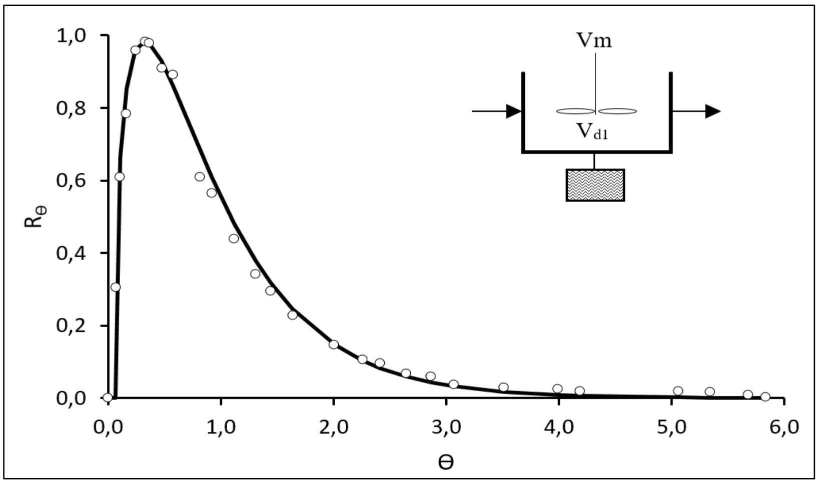

Figure 3: RTD curve for the stirred tank reactor with $R^2 = 0.96$, being (o) the experimental data and (-) the proposed model.
Source: Authors, (2020).

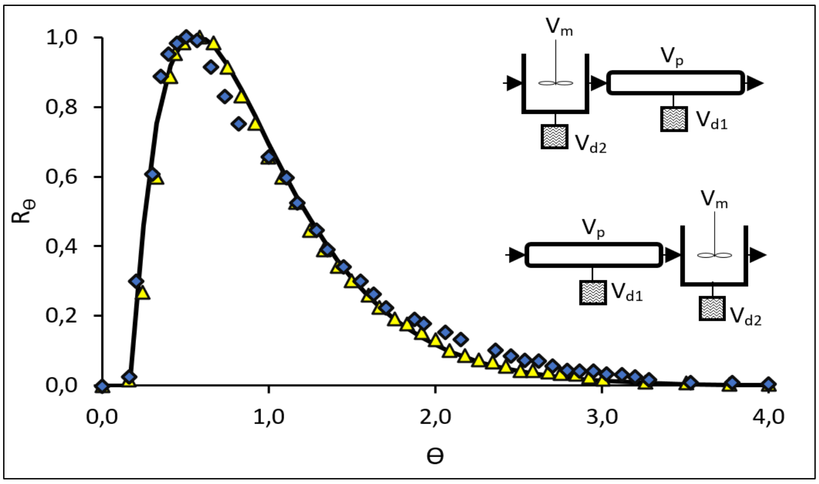

Figure 4: RTD curve for the RTA - RT and RT - RTA dispositions respectively, with $R^2 = 0.98$, being (Δ), (◊) the experimental data of the dispositions tested respectively, and (-) the proposed model.
Source: Authors, (2020).

This non-ideal flow model fits more than 96% regression coefficient in all cases, thus demonstrating the reliability of the results. The experiments carried out in the RT and RTA reactors individually and in their possible series arrangements demonstrate that the model is applicable, novel and useful for the studied non-ideal flow condition.

Unlike the models for ideal systems studied by Levenspiel [13] (**Erro! Fonte de referência não encontrada.**), the non-ideal flow model developed in this work, satisfactorily represents the deviations from the ideal flow characterized by the presence of dead water in the reactors.

III.4 MATLAB® SIMULATIONS OF THE PROPOSED MODEL

Simulations performed in MATLAB® demonstrate the effectiveness of the model based on the dispersion number for «open systems», both for the experiences carried out and for the extreme conditions where the tracer could behave as plug flow when D/uL→0 or complete mixing when D/uL→∞ (**Erro! Fonte de referência não encontrada.**).

The RTD curves shown in **Erro! Fonte de referência não encontrada.** are extrapolated and comparable (showing the same trend) with those reported by Levenspiel [14] (**Erro! Fonte de referência não encontrada.**).

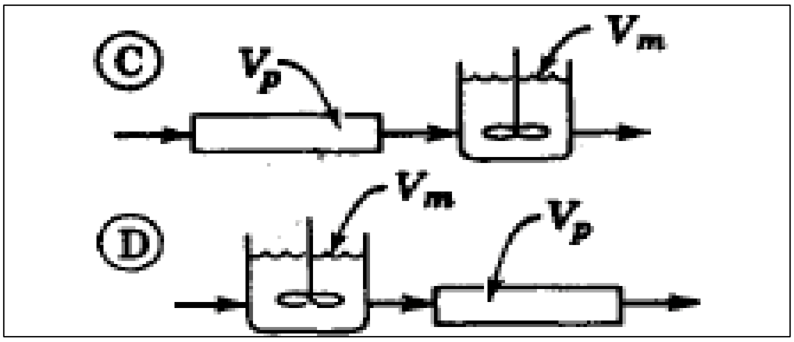

Figure 5: Ideal flow model proposed by Levenspiel.
Source: [13].

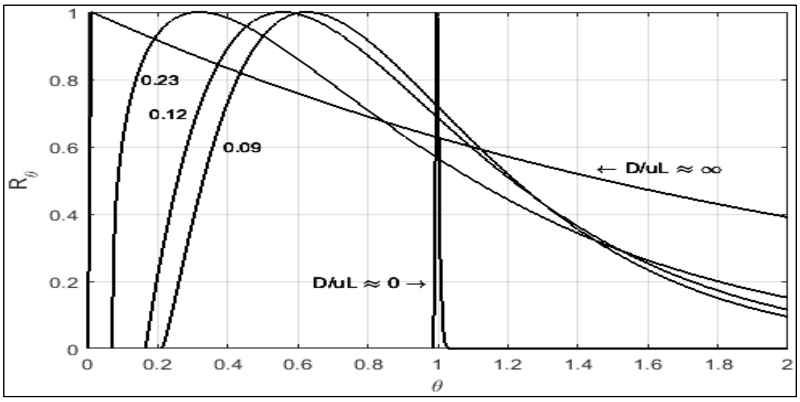

Figure 6: Simulations performed in MATLAB® of the RΘ vs Θ Curve for open systems with different back mix intensities (D/uL) predicted by the proposed model.
Source: [14].

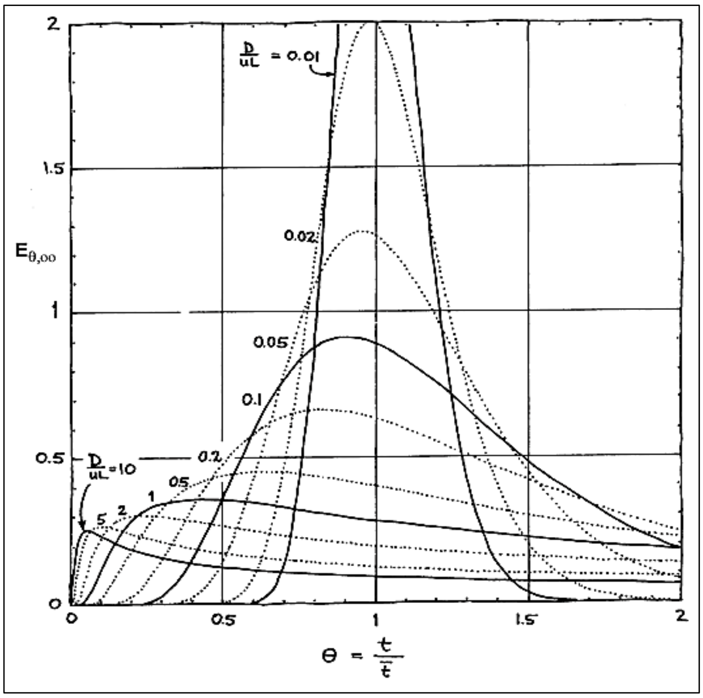

Figure 7: Dimensionless response for open-open boundary conditions as reported by Levenspiel.
Source: [14].

III.5 DEAD WATER FRACTIONS ANALYSIS

Table 1 shows the dead water fractions obtained for the RT, RTA systems and their serial arrangements; as well as those predicted according to the developed mathematical model. Furthermore, the error between the experimental and theoretical data is reported.

As can be seen, the order in which the reactors were combined does not exert a marked influence on the total fraction of stagnant regions, since for the two arrangements studied this value remains practically constant.

Table 1: Dead water fraction for the studied cases: RTA, RT and their serial arrangements.

	Dead water fraction (f_{Vd})			
	RTA	**RT**	**RTA-RT**	**RT-RTA**
System	0.1646	0.0507	0.0671	0.0699
Model	0.1265	0.0422	0.0551	0.0551
Error	0.0381	0.0085	0.0120	0.0148

Source: Authors, (2020).

This result is characterized by very similar Residence Time Distributions as observed in Fig. 4. As expected, the volumes of dead water in the stirred tank reactor are greater than in the tubular reactor, conditioned by the above characteristics geometric and flow of reactors. The developed mathematical model predicts dead water values well in all cases, with small estimation errors.

IV. CONCLUSIONS

As a result of the experiments to characterize the behavior of the flow through a stirred tank reactor and a tubular reactor and their series combinations, it is concluded that the order in which the tubular reactor and the stirred tank reactor are connected does not influence the flow model of the system, this being the same for the two combinations studied.

Unlike the ideal system reported in the literature, in the studied system there are dead water regions in both reactors and it is concluded that the residence time distribution curves are coincident for the possible series dispositions, as in the case of reactors with ideal behavior. The obtained mathematical model presents a good fit to the experimental data and describes the RTD curves for the systems studied with dead water. It was shown that for the combination of a series RT and RTA, the model that describes its behavior corresponds to a series with dead water in both equipment and that, although the arrangement changes, the RTDs are the same. The sum of the dead water fractions from the series of a tubular reactor and a stirred tank reactor are practically independent from the equipment arrangement. The simulation of the system using the model obtained and the MATLAB® software allowed analyzing the variations that occur in RTDs when the degree of backmix changes in the studied system. A similar behavior to that reported for open-open systems was found.

V. AUTHOR'S CONTRIBUTION

Conceptualization: Iván Leandro Rodríguez Rico and Roberto Jesús Cabrera Carrazana.
Methodology: Iván Leandro Rodríguez Rico and Roberto Jesús Cabrera Carrazana.
Investigation: Iván Leandro Rodríguez Rico, Roberto Jesús Cabrera Carrazana and Yeslié González Bermúdez.
Discussion of results: Iván Leandro Rodríguez Rico and Roberto Jesús Cabrera Carrazana.
Writing – Original Draft: Iván Leandro Rodríguez Rico.
Writing – Review and Editing: Iván Leandro Rodríguez Rico and Roberto Jesús Cabrera Carrazana.
Resources: Roberto Jesús Cabrera Carrazana.
Supervision: Roberto Jesús Cabrera Carrazana and Yeslié González Bermúdez.
Approval of the final text: Iván Leandro Rodríguez Rico, Roberto Jesús Cabrera Carrazana and Yeslié González Bermúdez.

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