Model of a Laboratorial Tubular Reactor by the Determination of the Distribution of Residence Times

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Introduction

The analysis of the residence-time distribution (RTD) for a given reactor can bring important information to diagnose the reactor operation and identify flux problems, to model the reactor when some physical properties are not available, or to predict some properties of the outlet stream that depend on the reactor residence time, such as concentration, conversion or selectivity.

The present work was divided into two parts: in the first part the experimental RTD of a tubular reactor with 350 mL was determined for two different flow rates and a model of the reactor was obtained. In the second part the reaction of persulfate with iodide was performed in the same reactor to determine the experimental conversion and compare it to the theoretical conversion given by the ideal plug-flow reactor (PFR) model and the RTD model.

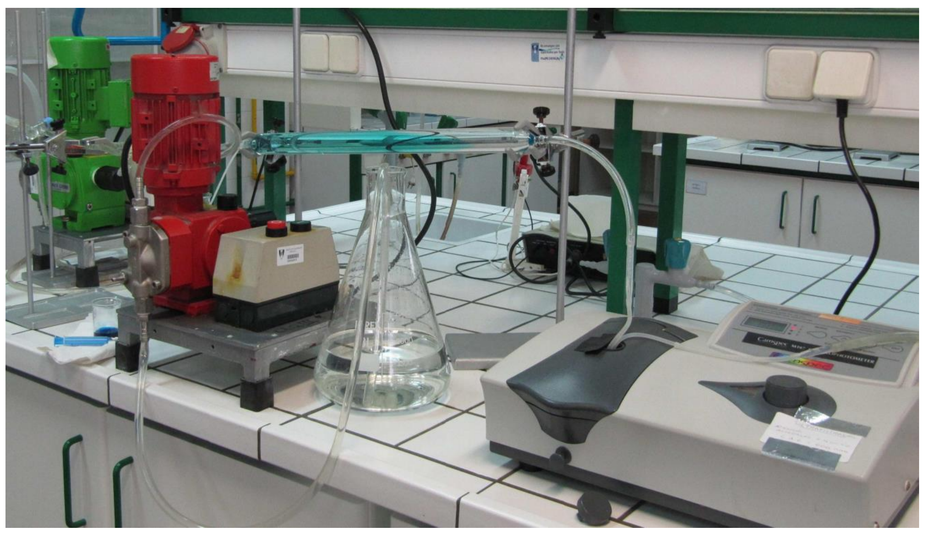

Figure 1. Photograph of the experimental installation for the determination of the experimental DTR.

Determination of the Experimental RTD

The experimental RTD of the tubular reactor was obtained by the injection of methylene blue through a pulse input at the entrance of the reactor while the absorbance of the outlet stream was measured using a spectrophotometer.

Due to the proportionality between the concentration and absorbance, assuming valid the Lambert-Beer Law, in a pulse input the time distribution function can be related to the trace concentration/absorbance according to:

$$RTD(t) = \frac{C(t)}{\int_0^\infty C(t)dt} = \frac{A(t)}{\int_0^\infty A(t)dt}$$

In Figure 2 the obtained experimental RTD's are presented together with the expected RTDs for the ideal plug-flow reactor at the two flow rates.

The possibility of the existence of bypass was excluded, since the tracer took a considerable amount of time to be detected, $Q = Q_{effective}$. In the second consistency test, the average residence time, $\bar{t}$, was calculated in order to determine the effective reactor volume, $V_{effective}$, and with that the dead volume, V_{dead}, inside the reactor. Calculating the variance, σ^2, allows to have an idea of the degree of macromixing inside the reactor, for and ideal PFR σ^2 should be equal to zero. The results are exhibited in Table 1.

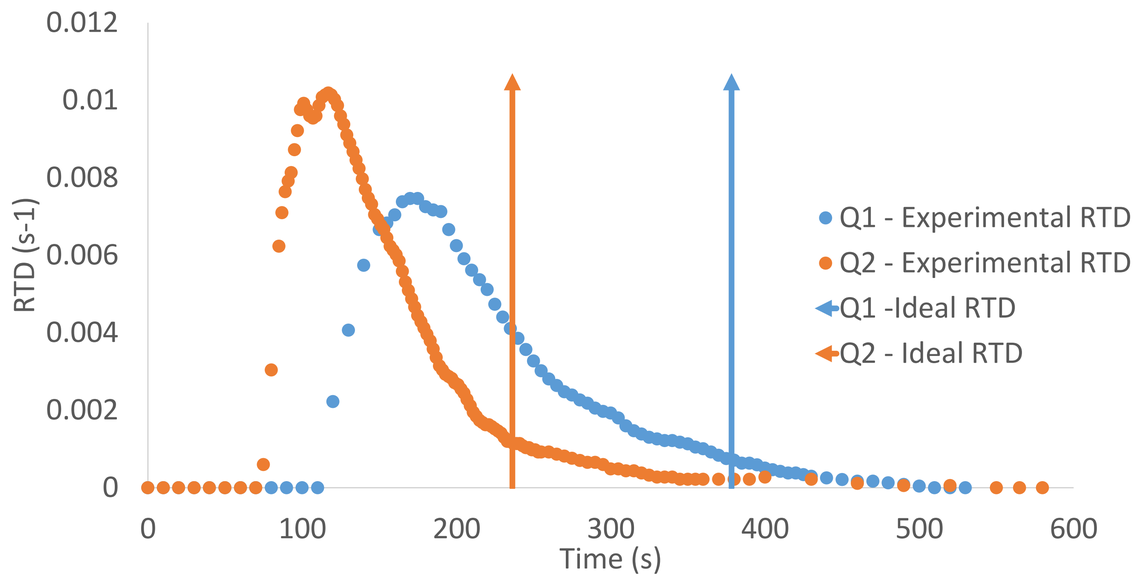

Figure 2. Experimental DTR compared with the ideal reactor DTR.

Table 1. Experimental results.

	θ (min)	$\bar{t}$ (min)	$V_{effective}$	V_{dead}	σ^2
Q_1=55.5 mL/min	6.31	3.61	200 mL	150 mL	5075
Q_2=88.9 mL/min	3.94	154	228 mL	121 mL	4644

Reactor Modelling

The descriptive model of the reactor was developed considering the RTD for a piston flow reactor (PFR) with a battery of continuous stirred tank reactor (CSTR) in series. The DTR for this type of association is described by the following equation:

$$RTD(t) = \begin{cases} 0 & \text{for } t < t_1 \\ \frac{(t-t_1)^{n-1}}{(n-1)!\,t_2^n} e^{-\frac{t-t_1}{t_2}} & \text{for } t \geq t_1 \end{cases}$$

The number of CSTRs, n, and the PFR and CSTR's residence times, t_1 and t_2, respectively, were estimated using *gPROMS*® Parameter Estimation tool by reducing the deviations between the experimental points and the ones predicted by the model.

The adjustment resulted in an association of a PFR with two CSTRs in series, Figure 4. Table 2 presents the resultant estimated parameters and the average deviations for the two flow rates.

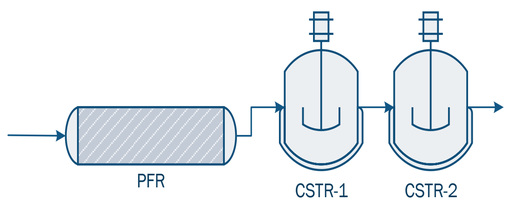

Figure 4. Representation of the reactors association.

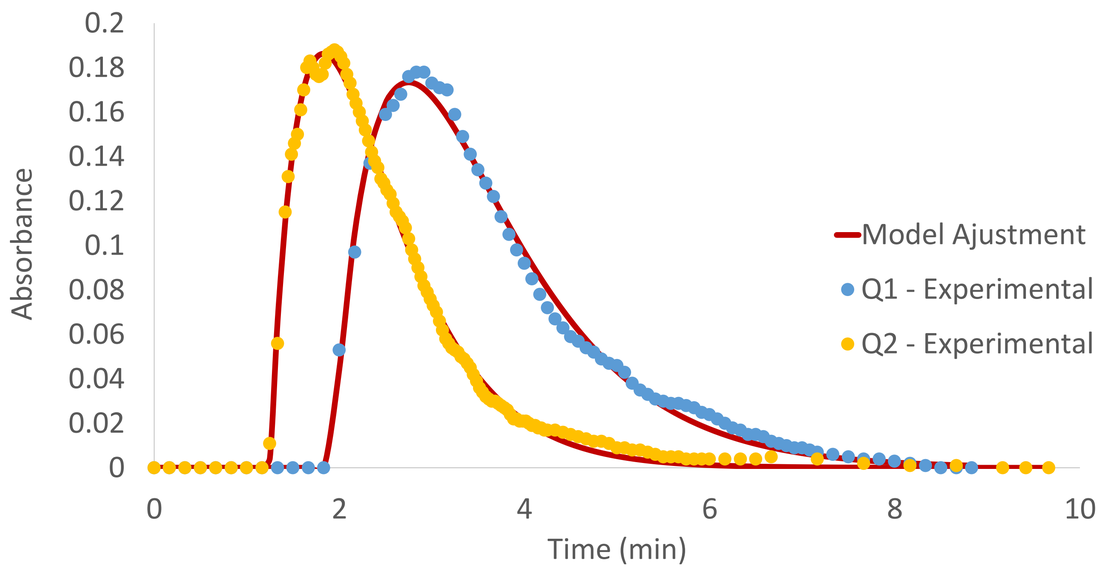

Figure 3. Experimental absorbance compared with model fitting.

Table 2. Adjustment results.

	n	t_1 (min)	t_2 (min)	Av. Dev.
Q_1	2	1.91	0.84	0.32 %
Q_2	2	1.24	0.58	0.27 %

Prediction of the Conversion

The reaction of persulfate with iodide is described by the following equation: $S_2O_8^{2-} + 2I^- \rightarrow I_2 + 2SO_4^{2-}$

Using the total segregation premise, the average concentration of the limiting reactant at the exit of the reactor can be obtained by means od the RTD according to:

$$\overline{C_A}(t) = \int_0^\infty C_A^*(t)DTR(t)dt$$

Where $C_A^*(t)$ is the concentration of the limiting reactant in a BATCH reactor. Table 3 presents the conversion results obtained for a flow rate ≈ Q_1 and compared to the theoretical conversion in an ideal PFR and by the DTR, assuming total segregation.

Table 3. Conversion results.

$S_2O_8^{2-}$ Conversion	
Experimental	23.5%
Ideal PFR	28.2%
Total segregation	23.3%

Conclusions

- A descriptive model based on the distribution of residence times was successfully accomplished.
- The real reactor presents a typical behavior of a Piston Flow Reactor with a considerable macro-mixing degree.
- This is a good example of a gPROMS application that can be use during the academic curriculum.

References

[1] F. Lemos, J. M. Lopes, and F. R. Ribeiro, "Reactores Químicos" *IST Press, 2002, 1st Ed.*

Acknowledgments

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