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Chemical Modeling of a Photocatalytic Reactor of Spiral Geometry

Fateh Naitali* and Hafida Ghoualem

Laboratory of Electrochemistry-Corrosion, Metallurgy and Inorganic Chemistry. Faculty of Chemistry. University of Sciences and Technology. Houari Boumediene. Box N°32 El-Alia. Bab-Ezzouar. Algiers. Algeria.
*hghoualem@usthb.dz, *fatehnaitali@yahoo.fr*

ABSTRACT

Many reactors are used in catalytic reactions. Modeling reactors have a great importance before there used in industrial applications or anywhere application.
The injection of a chemical tracer into the reactors is a conventional technique allowing the characterization of the hydrodynamic flow, the connections between the injection point and the fluid outlet point, the circulating fluid flow rates between these points and the volumes of fluids located between these points.
The objective of this work is the modeling of a photo catalytic reactor of spiral geometry by the method of the distribution of the residence times.
The modeling of the reactor is based for the geometry of the reactor and the hydrodynamics of the liquid.

Key words: Photocatalytic reactor, spiral geometry, modeling, distribution of the residence times

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INTRODUCTION

To create a conventional chemical reactor model, all the phenomena and processes present in this reactor must be identified and described.
The mathematical description of this model which usually contains laws of chemical, physical and physico-chemical conservation of the process is expressed with a set of deterministic equations (algebraic, differential).
All the constants that appear in these equations, are called the model parameters, and have a physical meaning because they characterize the appropriate process or phenomenon.
The method of distribution of residence times (DRT) via the tracing technique is widely used to characterize the hydrodynamic regime and the reaction kinetics in chemical reactors.
The tracing technique consists in temporarily injecting a chemical tracer at the inlet of a reactor and registers its restitution in the output stream.
Many researchers [1-4] are interested for the study of catalytic reactions in different form reactors.
The aim of this work is to model a photo catalytic reactor of spiral geometry by the method of the distribution of residence times (DRT).

MATERIALS AND METHODS

The reactor studied has a spiral shape of 10 mm in outer diameter, 8 mm in internal diameter, 100 mm in turn diameter, 1500 mm in length and 175 mL in volume.
The experimental setup used is shown in fig. 1.

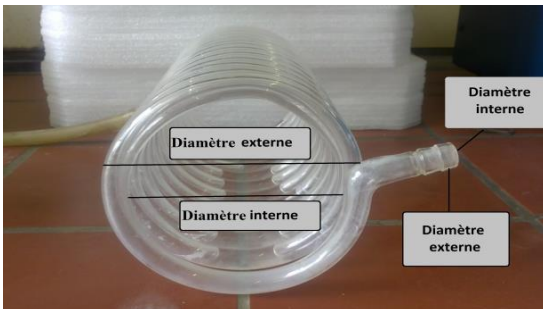

Fig. 1 Spiral reactor studied.

For the hydrodynamic modeling, two flow rates were studied (20.51 and 29.104 mL / s) in three different fluid circulation positions (horizontal, bottom to top and top to bottom).

The reactor modeling required the estimation of several hydrodynamic parameters such as:

Residence time (ts), variance (σ) number of Reynold (Re), number of peclets (Pe), number of dean, axial diffusion coefficient, Axial scattering coefficient (Dax) molecular diffusion coefficient (Dm), accessible volume **(**Vacc**)**, dead volume (Vm), pressure drop coefficient, pressure drop, prediction of conversion in an RCPA , ratio between the instability frequency ft and the strouhal frequency and friction factor (F).

Residence time (ts)

$$ts = \frac{\sum_{0}^{\infty} t_{si} C_i(t_{si}) \Delta t_{si}}{\sum_{0}^{\infty} Ci(t_{si}) \Delta t_{si}} \quad (1)$$

$ts^2 = \sum t^2_i \,.C(t\,i)\,.\,\Delta t_i \,/\, \sum C(t_i)\,.\,\Delta t_I$ and $(ts)^2 = \left(\frac{\sum_{0}^{\infty} t_{si} C_i(t_{si}) \Delta t_{si}}{\sum_{0}^{\infty} Ci(t_{si}) \Delta t_{si}}\right)^{\wedge}2$

Variance (σ)

$\sigma=(ts^2-(ts)^2)$ (2)

Number of Reynolds (Re)

$Re = \frac{\rho\, U\, D}{\mu}$ (3)

Number of Peclet (Pe)

$Pe=2/(\sigma^2/(ts)^2)$ (4)

Axial scattering coefficient (Dax)

This parameter represents the deviations of the liquid flow with respect to a piston flow, the axial retro-mixing and the velocity profile. Axial dispersion can be described by:

$Dax = \frac{U\,L}{Pe}$ (5)

Molecular diffusion coefficient (Dm)

This coefficient is calculated by the following equation:

$Dm=Dax-\frac{U^2 d^2}{192\ Dm}$ (6)

The number of perfectly stirred continuous reactors (RCPA) maching (J)

$J = (ts)^2 / \sigma^2$ (7)

Dead volume (Vm)

$Vm\ (\%)= (1 - \frac{ts}{\tau})\ .\ 100$ (8)

Accessible volume (Vacc)

Vr = Vm + Vacc and Vacc = Vr – Vm (9)

Coefficient of pressure loss (Darcy's relationship) and pressure loss (ΔP)

The coefficient of loss of load is given by: $\wedge=\frac{0,3164}{Re^{0,25}}$ (10)

The pressure drop is representative of the resistance to flow in the medium.

$\Delta P = \frac{L}{2\,d} . \wedge . \rho . U^2$ (11)

Prediction of Conversion into an RCPA (X) for 1st order reactions

$X(mol)=\frac{k.\tau}{1+k.\tau}$ (12)

Ratio of instability frequency ft to Strouhal frequency

$ft/fs=0.095Re^{0.5}$ (13)

Friction factor (F)

F= ^/4 (14)

Number of Dean « De ».

$De=Re.(dh/Re)^{0.5}$ ***[5]*** (15)

RESULTS AND DISCUSSION

Results of modeling of the operating regime of the reactor

Table 1 summarizes the different values calculated during the determination and modeling of the operating regime of the reactor.

Table -1 Values calculated during the determination and modeling of the operating regime of the reactor studied

Flow	**Q = 20.51 mL/s**			**Q = 29.104 mL/s**		
Fluid circulation	**from bottom to top**	**From top to bottom**	**horizontal**	**from bottom to top**	**From top to bottom**	**horizontal**
ts (s)	13.73	11.38	19.64	4.301	4.277	4.267
σ2=((ts)^2-(ts^2))	65.8871	10.6156	3.4104	78.058	2.070	83.239
Pe	5.72	24.40	226.21	0.47	17.67	0.44
n RPA J	2.86	12.20	113.10	0.237	8.8367	0.2187
Re	3260	3260	3260	4627.368	4627.368	4627.368
Dax	0.1069	0.0251	0.0027	1.8316	0.0491	1.9852
Dm	0.1069	0.0251	0.0027	0.0222	0.0901	0.0640
Vacc (mL)	102.08	109.82	90.80	132.03	131.65	130.40
To (S)	6.83	6.83	6.83	4.81	4.81	4.81
Vm/Vr (%)	50.29	40.03	65.25	10.57	11.07	12.73
Vm (ml)	37.92	30.18	49.20	7.97	8.35	9.60
ft/fs	0.5424	0,5424	0,5424	0,6462	0,6462	0,6462
Coeff of darcy	0.0418	0.0418	0.0418	0.0383	0.0383	0.0383
Loss of charge	0.652	0.652	0.652	1.2032	1.2032	1.2032
F(friction)	0.0104	0.0104	0.0104	1850.95	1850.95	1850.95
De	1304	1304	1304	0.0095	0.0095	0.0095

The parameters of the fluid flow in the reactor depend on its arrangement and the flow rate.

The longest residence time (ts) is equal to 19.64s for a small variance (σ2) equal to 3.41, a flow rate of 20.51 mL/ s for the horizontal position of the reactor.

The shortest ts equals 4.26 s corresponding to a high variance of 83.23, a flow rate of 29.104 mL / s for a horizontal position of the reactor.

The residence time and the variance σ2 were calculated by equating the integral signal with a sum sign.

The Renolds (Re) is greater than 3000 for the two flow rates studied. It is 3260 for the flow rate of 20.51 mL / s and 4627.368 for the flow rate of 29.104 mL / s.

The largest value of Peclet (Pe) is obtained for the flow rate of 20.51 mL / s and the horizontal position of the reactor. The lowest value is obtained for the flow rate of 29.104 mL / s for the horizontal position of the reactor.

For the axial and molecular diffusion coefficients (Dax and Dm), they are equal to the flow rate of 20.51 ml / s irrespective of the position of the reactor.

For a flow rate of 29.104 mL / s, the Dax is larger than the Dm for the vertical (up-down) and horizontal position, but for the vertical position (bottom-up) it is the Dm that is greater than Dax.
The number of perfectly stirred continuous reactors (RCPA) (J) has a maximum of 113 reactors for the flow rate of 20.51 mL / s in the horizontal position of the reactor.
The average flow time is 6.83s for a flow rate of 20.51 mL / s and 4.81s for the flow rate of 29.104 mL / s.
The prediction of the conversion in an RCPA (X) for 1st order reactions is shown in the following figure.

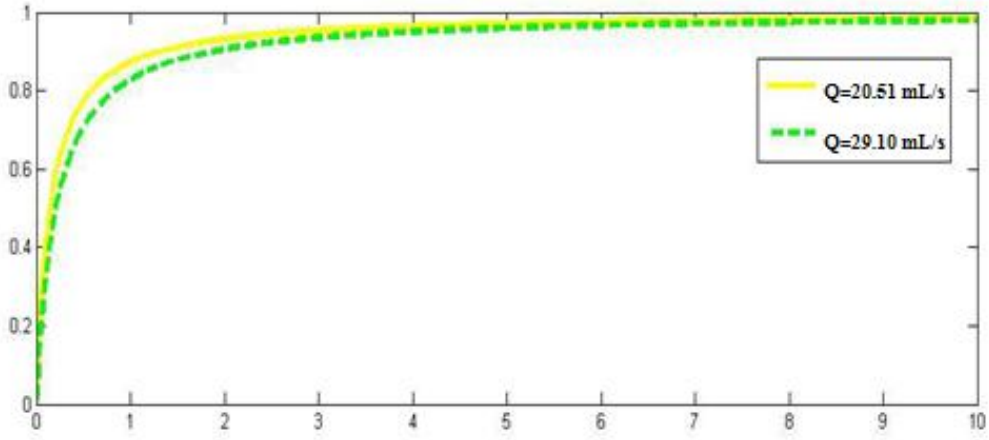

Fig. 2 Conversion Variations in an RCPA (X) for 1st order reactions

The conversion reaches the plateau after 4 hours for both flows.
The rate of conversion of the 20.51 mL / s rate is slightly higher than that of the rate of 29.104 mL / s.
The percentage of the dead volume is important, it is equal to 65.25% for the flow rate of 20.51 mL / s in the horizontal position of the reactor and it is equal to 10.57% for the flow rate of 29.104 mL / s in position (bottom up).
The pressure loss remains unchanged whatever the position of the reactor, but it varies according to the flow rate, it is greater for the flow rate of 29.104 mL / s than for the flow rate of the reactor. 20.51 mL / sec.
The friction factor (F) is greater for the flow rate of 29.104 mL / s than for the flow rate of 20.51 mL / s.
There is not much difference between the ft / fs ratios for the two rates where ft is the instability frequency and fs the Strouhal frequency.
The ratio is 0.54 for the flow rate of 20.51 mL / s and 0.64 for the flow rate of 29.104 mL / s.
Some researchers [6, 7] used friction factors equal to those found in monophasic as suggested by Wallis (1966) [8] for two-phase flows with a void fraction of less than 10. %.
Friction factors found experimentally, however, are much larger [9-11].

Hydrodynamic parameters of the reactor
Calibration curve

The electrical conductivity calibration curve of in tracer (H_3PO_4) is recorded over time at the outlet of the reactor.
The results obtained are shown in the following figure.

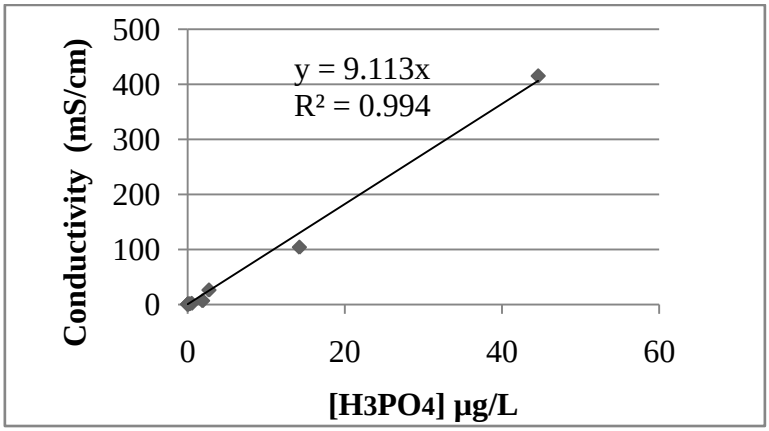

Fig. 3 Calibration curve of tracer conductivity as a function of concentration

Distribution of residence time

The determination of the residence time distribution has been considered for two flow rates.

- Flow rate equal to 20.51mL / s.

The distribution of the residence time in the reactor at different positions for a liquid flow rate of 20.51 mL / s flow rate of 20.51 mL / s is grouped in Fig. 4.

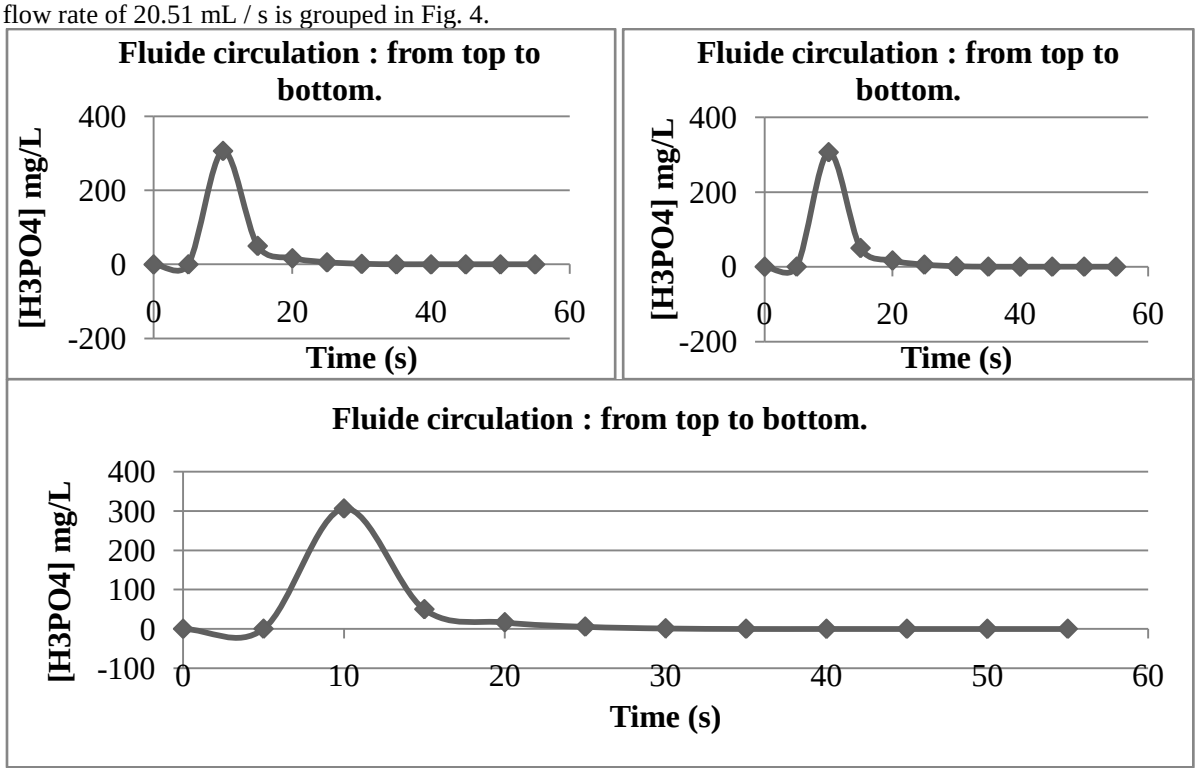

Fig. 4 Evolution of the DTS in the reactor at different positions for a liquid flow rate of 20.51 mL /s.

As for the straight channel, the flow is closer to a piston flow when the reactor position is horizontal.

By comparing the shape of the output signal of the three distributions of the residence times, it is observed that in the vertical position, the flow detaches from the piston flow.

The spiral reactor behaves in each circulation as a piston-type reactor, characterized by low axial dispersion irrespective of the flow rate, which makes it industrially interesting.

- Flow rate equal to 29.104 mL / s.

The residence time distribution (DRT) in the reactor at different positions for a liquid flow rate of 29.104 mL / sec is in fig. 5.

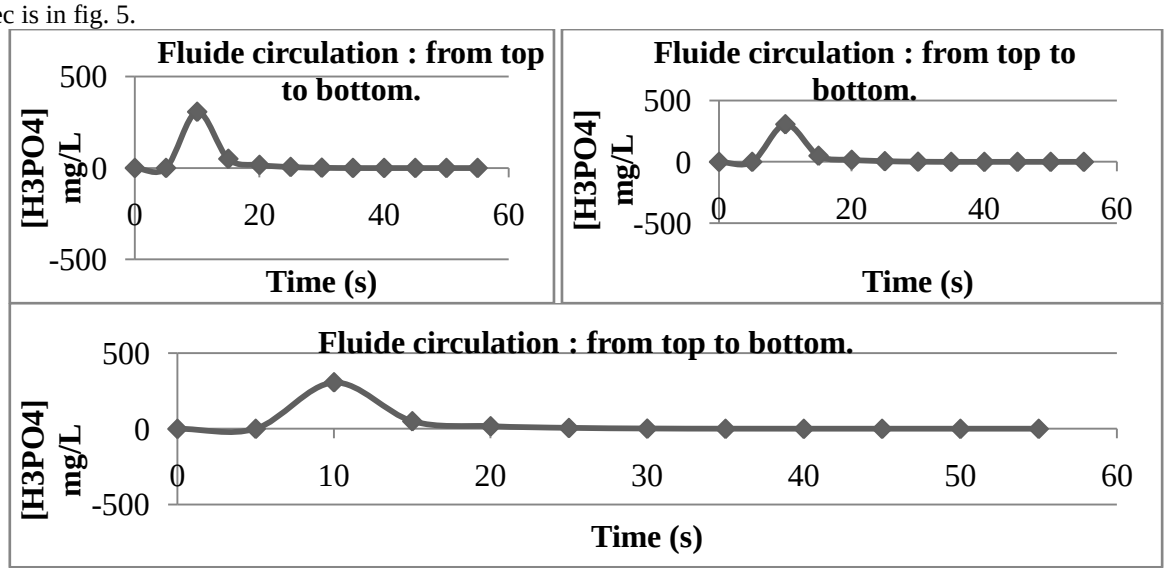

Fig. 5. Evolution of the DRT in the reactor at different positions for a liquid flow rate of 29.104 mL / s.

As for the straight channel, the flow is closer to a piston flow when the reactor position is horizontal.

By comparing the shape of the output signal of the three distributions of residence times, it is observed that the flow is of the piston type whatever the position of the reactor.
Nevertheless, the position of the reactor influences the hydrodynamic forces which leads to a decrease in the fluid flow velocity.
A decrease in the feed rate increases the axial mixing and thus the dispersion of the DRT signal. The flow then moves away from that of a piston reactor [12].
The flow deference as a function of reactor position is explained by the dynamics of tracer clouds and the hydrodynamic forces exerted on them.
A study [13] concludes that cloud dynamics may be the main cause of the transition between flow regimes.
This transition occurs at much higher gas flows in Pairlift than in a bubble column [14] due to the flow of liquid.
In addition, the velocity of the liquid increases with the height of the reactor [15, 16].

CONCLUSION

Very widely used today in the characterization of chemical reactors, the technique of distribution of residence times (DRT) is very useful for characterizing the hydrodynamic regime and highlighting the presence of geometrical defects in the reactors and model the non-ideality of flows [17].
The results obtained show that:
As the speed of the liquid increases, the residence time decreases.
If the average residence time decreases and the number of perfectly stirred reactors increases, the volume of each perfectly stirred reactor must be smaller, so that the flow approaches more than a piston-dispersion flow. The existence of several small backmixing zones between the particles causes all of these zones to act as a large series of perfectly stirred reactors and thus, the flow becomes closer to a piston flow.
If these areas are larger and small in the reactor, the associated backmix will have a negative impact on the flow and move away from the piston flow [18].
The dimensionless numbers depend on the flow rate and the position of the reactor, which is explained by the influence of the porosity of the reactor walls. Indeed, the porosity in the turns is greater than that of the rectilinear channel, which may imply that, because of the larger empty volume, the flow regimes will have a greater impact on the recirculation zones of the liquid at different positions. of the reactor. The pressure drop of the liquid in the reactor for the flow rate of 29.104 mL / s is greater than that observed for the flow rate of 20.104 mL / s. This increase in pressure loss can be explained by the higher surface velocities of the liquid and the decrease in the equivalent diameter due to the wall surface.
Circulation velocity affects turbulence, heat transfer coefficient between fluid and reactor wall, liquid gas transfer and shear forces [19].
Modeling by dimensionless numbers shows that Q = 20.51 mL / s in horizontal arrangement. Hydrodynamic modeling is consistent with modeling by dimensionless numbers.
The variations of the DTS as a function of the position of the reactor photo can be explained by the influence of the inertial forces which can act on the acceleration and / or slowing of the fluids in the bed of particles.
The deviation from ideal piston flow increases due to disparity in local velocities. Indeed, the hydrodynamics of the flows in a spiral-geometry reactor has a great influence on the performances of this reactor but remains difficult to predict with precision.
The flow regimes, the loss of pressure, the retention rate and the axial dispersion of the liquid phase are hydrodynamic parameters necessary to understand this type of reactor.
It therefore appears as a system well suited to photo catalytic reactions. The prediction of the conversion shows that after 5 hours of treatment the plateau is reached hence the choice of photo-catalytic treatment for 5 hours.

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