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Study the variables of Esterification Reaction of Acrylic acid with Butanol and Comparative with the Simulation

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Abstract

Esterification is the general name for a chemical reaction in which two reactants (typically alcohol and acid) form an ester as the reaction product and water.
Butyl acrylate, which can be produced in liquid phase from butanol and acrylic acid, is an important chemical industry where it is used in the production of coating and inks, adhesives, sealants, textiles and plastics. The reaction equilibrium and the kinetics of the butyl acrylate synthesis catalyzed.
The present work considers the reaction between butanol and acrylic acid over different operating parameters (feed flow rate, temperature, and length of reactor) to get the best conversion of butyl acrylate.
In addition, the tubular reactor which using in this study is designed in the lab. The chemical process which done in the lab by tubular reactor, has been simulated in standard commercial software (HYSYS) with the same parameters and variables. The comparative between the experimental results and the simulation results were very similar and closed.

Keywords — Estrifiaction , Butayle Acrylate , Simulation , Plug Flow Reactor (PFR).

1. Introduction

Esterfication reaction is the important reaction in industry field which product different kinds of esters throughout add ALCKHOL and ACID to get ester and water as production.
One of the esters is Butyle acylate , which produced by reverse reaction butanol and acrylic acid .
Acrylates (acrylic acid esters) are important precursors for varnishes adhesives , coatings , leather, plastics and textiles [1].
The main reaction described by this equation:-

$$CH_3 - (CH_2)_3 - OH + CH_2 = CH - COOH \leftrightarrows C_4H_9 - O - CO - CH = CH_2 + H_2O$$

The reactor which used in this study was Plug flow reactor (PFR), The presence of (Amprlyst 15) is used as a catalyst in the reactor to produce a butayl acrylate .
The previous studies about the esterfication are limited for butyl acrylate production, Stefan Schwarer and Ulrich Hoffmann (2002), Thay studied the same reaction of esterfication to produce a butayle acrylate and made simulation to compare the results after deal with the kinetics and reaction equilibrium but by different kind of catalyst [2].

The main objectives are study the variables that effect on Butyl acrylate production such as feed flow rate, temperature and reaction zone length. Additionally, the results of experimental work has been compared with simulation of HYSYS software results.

2. Experimental work

The reaction is prepared by (PFR) which is tube has 1.6 cm diameter contains an amount of catalyst (Amprlyst 15). The reactor is inside the thermal furnace with heating control system.
The diagram below explains the experimental work set up that contain 1.6 cm installed in the furnace. The feed stream composition (acrylic acid and butanol 1:1) supplied to tubular reactor by frequency pump.

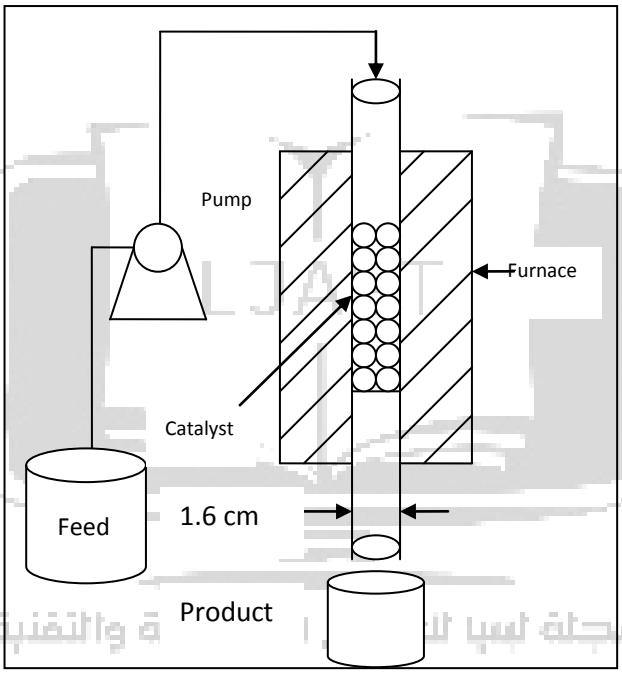

Fig.1 Diagram of plug flow reactor.

At start , the temperature inside the reactor set at 90 °C, the length of reaction zone is 1.6 cm and the flow rate of reactants is 0.5 mL/min.
Once the reactants touch the surface of catalyst, the reaction start and going to produce ester
After the first run as above specification, changed the variables like following table:

Table 1 Margin specifications

Temperature (°C)	Flow rate (mL/min)	Length of reaction zone (cm)
90	0.5	16
100	0.75	18
110	1	20

All the parameters have changed at each run of reactor and got different results of conversion of butyle acrylate .

3. Simulation

In this part, it has been simulated the experimental work by HYSYS software with the same fixed operation condition (feed composition and dimension of reactor).
The changing of results for conversion, temperature, flow rate and length of reaction zone reflects on the change in simulation condition as same as experimental work [3].

4. Results and discussion:

4.1 Results of experimental work:

Through the experimental work in the laboratory and study of a reaction between alcohol (Butanol) and the acid (Acrylic acid) to produce butyle acrylate and water.
When the samples have taken in each run, the parameters such as flow rate , temperature and weight of catalyst have been changed and then made a titration procedure of the samples[4] , also all the results obtained in the following tables of results:

Table 2 Results of Experimental Work

At 90°C		
Flow rate (lit/min)	Length of reaction zone (cm)	Conversion %
0.0005	16	16.40
	18	19.00
	20	21.90
0.00075	16	17.00
	18	21.10
	20	24.60
0.001	16	11.60
	18	17.00
	20	18.20
At 100°C		
Flow rate (lit/min)	Length of reaction zone (cm)	Conversion %
0.0005	16	28.10
	18	35.80
	20	40.70
0.00075	16	26.00
	18	27.70
	20	30.10
0.001	16	24.00
	18	27.00
	20	28.05

At 110°C		
Flow rate (lit/min)	Length of reaction zone (cm)	Conversion %
0.0005	16	32.70
	18	41.10
	20	43.60
0.00075	16	29.00
	18	37.40
	20	42.00
0.001	16	28.50
	18	36.00
	20	40.60

From the tables above, it observed the difference of percentage of conversion. As shown the conversion increases with the increasing of an amount of catalyst. From another side, the conversion will be decrease with increasing of flow rate of feed. Generally, the conversion of product will be increase with increase of temperature of reaction. The following curves show the results of experimental work.

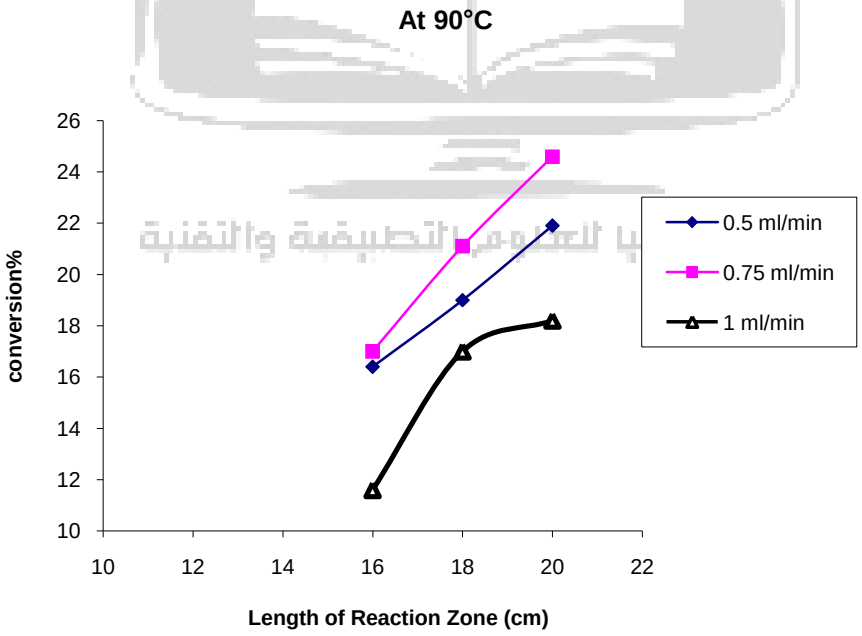

Fig 2 Conversion profile with the length of reaction zone at 90°C

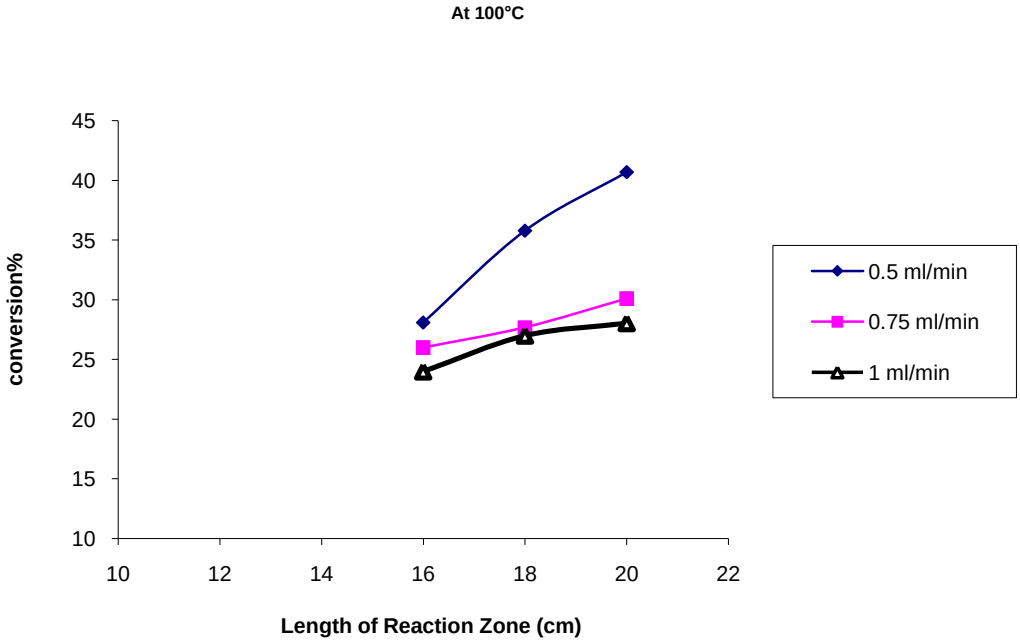

Fig 3 Conversion profile with the length of reaction zone at 100°C

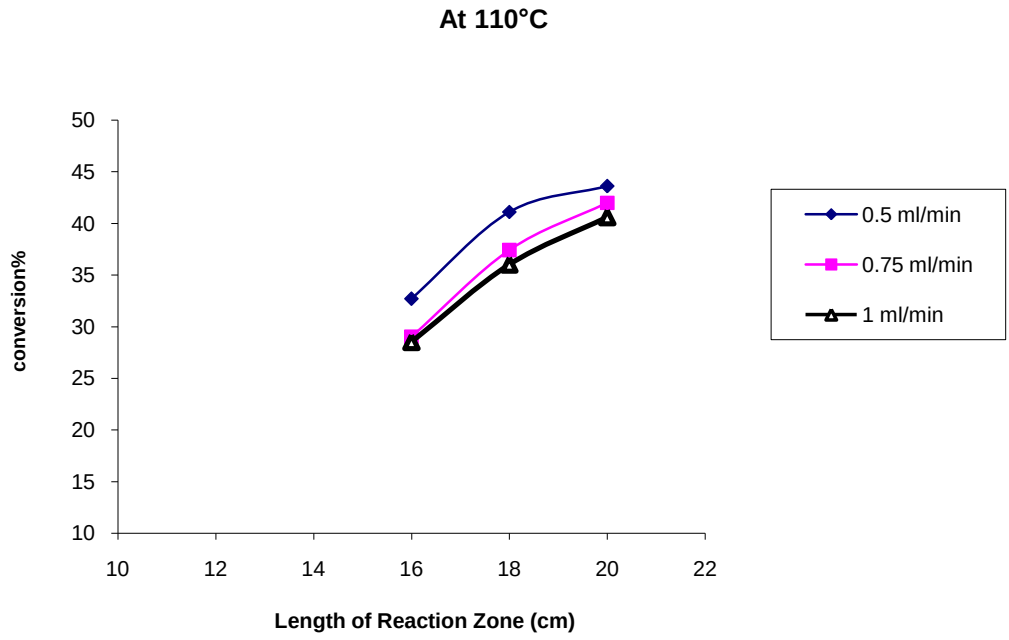

Fig 4 Conversion profile with the length of reaction zone at 110°C

4.2 Results of simulation:

The next tables explain the results of esterification reaction between butanol and acrylic acid under the same condition that applied in experimental steps.

Table 3 Results of Simulation Work

At 90°C		
Flow rate (lit/min)	**Length of reaction zone (cm)**	**Conversion %**
0.0005	16	18.8
	18	20.56
	20	22.24
0.00075	16	13.96
	18	15.37
	20	16.73
0.001	16	11.11
	18	12.28
	20	13.42
At 100°C		
Flow rate (lit/min)	**Length of reaction zone (cm)**	**Conversion %**
0.0005	16	30.17
	18	32.51
	20	34.66
0.00075	16	23.38
	18	25.43
	20	27.35
0.001	16	19.1
	18	20.9
	20	22.59
At 110°C		
Flow rate (lit/min)	**Length of reaction zone (cm)**	**Conversion %**
0.0005	16	43.64
	18	46.18
	20	48.42
0.00075	16	35.67
	18	38.17
	20	40.43
0.001	16	29.66
	18	31.99
	20	34.15

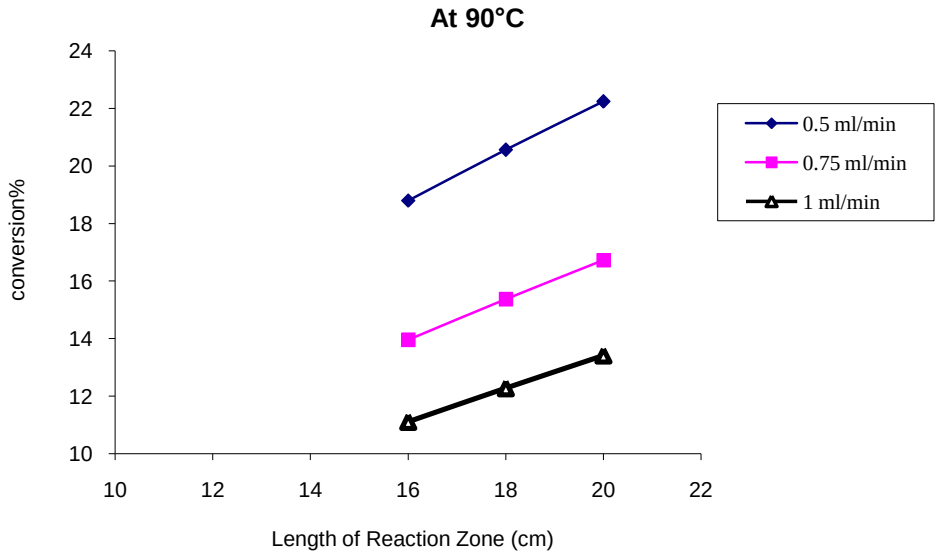

Fig 5 Conversion profile with the length of reaction zone at 90°C

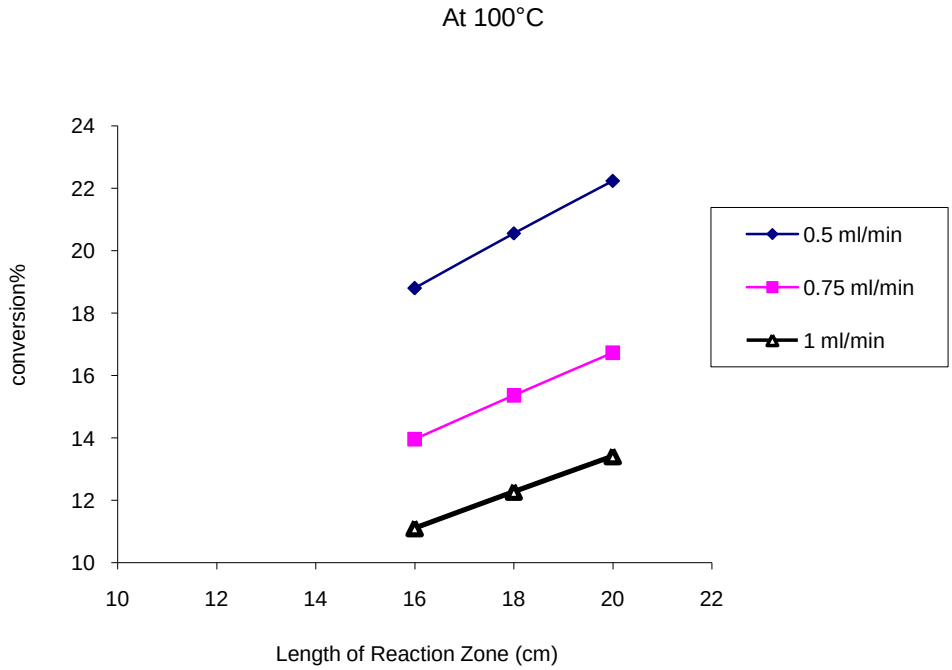

Fig 6 Conversion profile with the length of reaction zone at 100°C

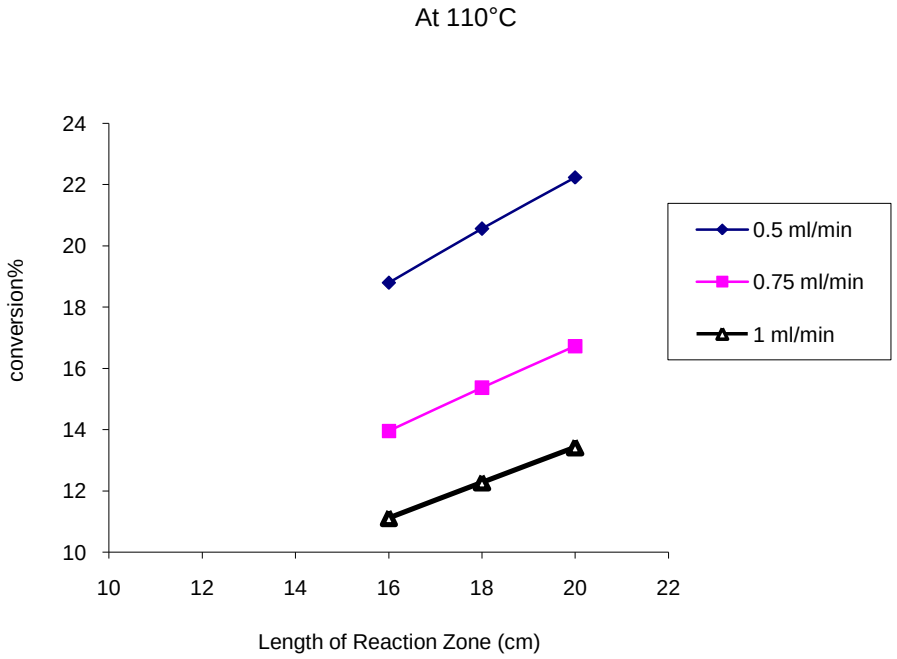

Fig 7 Conversion profile with the length of reaction zone at 110°C

4.3 Discussion

From the curves above which explain the conversion percentage of butayl acrylate, the conversion increase with the amount of catalyst. Therefore, the quantity of catalyst means more surface area for reaction and that leads to increase of conversion of product.
Also, from previous results, increase the flow rate of reactants lead to more quick pass due the catalyst which means there is not enough time to make well reaction with reactants.
In addition, the results of tables above explain that the conversion change with a temperature increasingly.

The reaction of esterification in the liquid phase and in the lowest boiling point of reactants is 117 ºC and these experiments are being conducted at temperatures of 90, 100,110 ºC, this step interaction remains in the liquid phase, but the products from this reaction are ester and water, as known, that the water evaporates at a temperature of around 100 ºC So, when temperatures 100, 110 ºC, the reversible interaction decreases significantly and leads to increase the conversion to more than 40%.

4.4 Experimental and Simulation Comparative:

The curves below show the conversion profile with the length of reaction zone at different reactor temperature (90, 100, and 110) ºC and same feed flow rate 1ml/min.

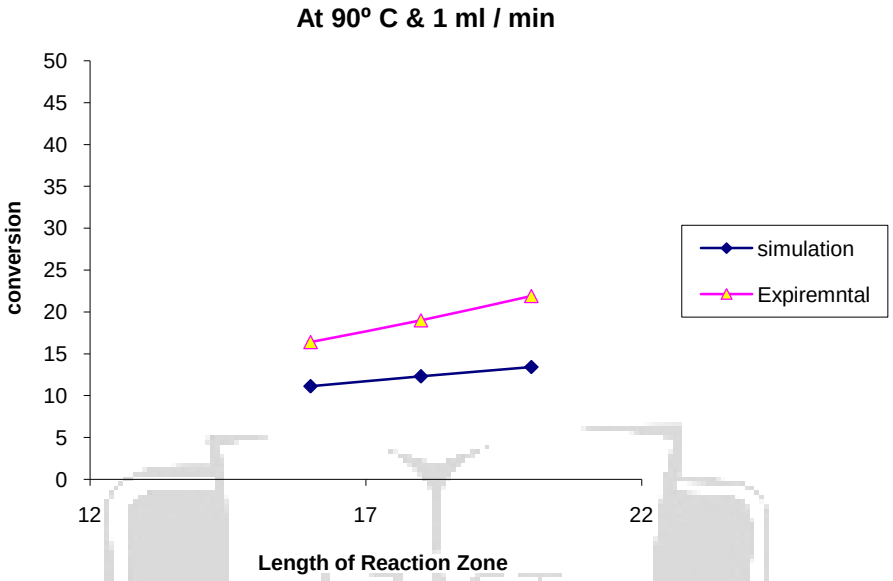

Fig 8 Experimental and simulation at 90°C

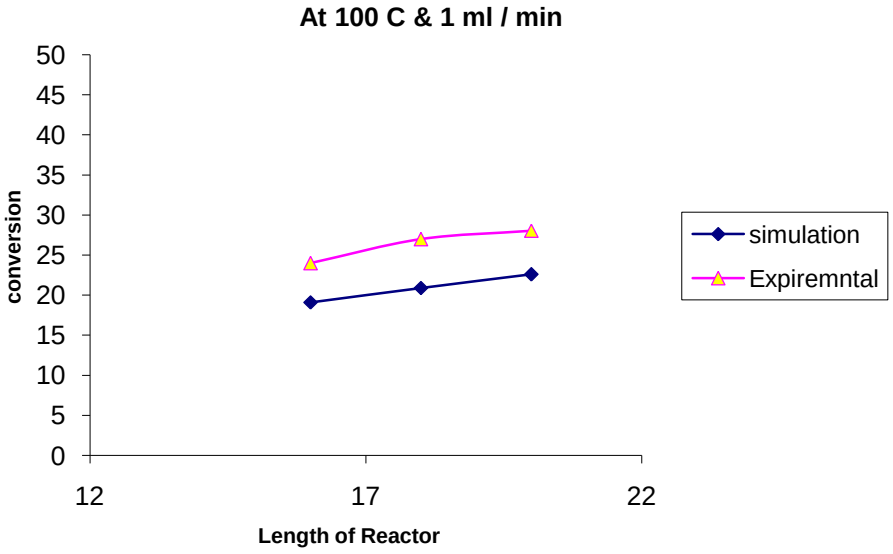

Fig 9 Experimental and simulation at 100°C

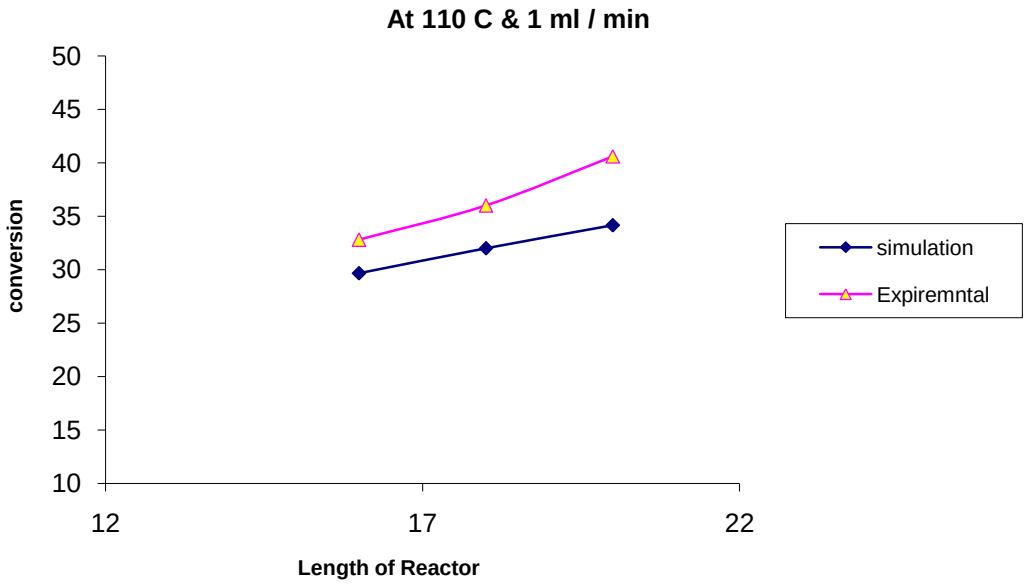

Fig 10 Experimental and simulation at 110°C

5. Conclusion:

- The main purpose of this work is study the variables that effect on Butyl acrylate production such as feed flowrate, temperature and reaction zone length.
- Temperature and length of reaction zone effect on the conversion of butyl acrylate positively.
- In other side, the effect of flow rate on the conversion was negative effective.
- The results of this work obtained that the experimental work is similar to the simulation for butayl acrylate production.
- Hysys software provides accurate modeling of butyle acrylate production and follows the same behavior pattern for mechanism of reaction that happened in experimental work.

6. References

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