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Simulation to Production of Styrene by Catalytic Dehydrogenation of Ethyl Benzene

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***Abstract*:** Petrochemical industries consider one of the most important industries in Pliocene which the most complex compound are manufactured such as styrene. Styrene is one of an important monomer in the industries of thermoplastic, 65% of all styrene used to produce polystyrene. Polystyrene is used in a huge range of everyday products and can be found in packaging, plastics, toys, consumer electronics ...etc.

The objective is to design a chemical plant to produce styrene by the catalytic dehydrogenation of ethylbenzene, taking ethylbenzene 180 kmol /hr as a base.

Preliminary material balance was made for the process to determine the total flow in the process. A simulation for the process was created in HYSYS software is used to study material balance in calculation the amount of material used and compared the results with the hand calculation.

Keywords- *Styrene Production from Ethyl Benzene*

I. INTRODUCTION

Styrene is a colorless, aromatic liquid. Nearly all of the commercial styrene is consumed in polymerization and copolymerization. This chemical serves as the basis for making polystyrene, a plastic that most people incorrectly refer to as Styrofoam (Styrofoam is polystyrene that has undergone a foaming process.) Polystyrene is used to make coolers, disposable coffee cups and a variety of other products that people use every day. However, technology that makes styrene primarily utilizes ethylbenzene. Styrene is an extremely important commodity chemical that has significant products and uses in our daily life. Thus, its manufacturing process has become the main topic of interest in this thesis. The two process routes that are used for styrene manufacturing are dehydrogenation and coproduction with propylene oxide. Nearly 90% of styrene production utilizes dehydrogenation, mainly because of its simplicity and cost-effectiveness.[1]

The styrene process was developed in the 1930s by BASF (Germany) and Dow Chemical (USA). Over 25×10^6 tons/year of styrene monomer is produced worldwide [2]. The annual production of styrene in the U.S.A. exceeds 6×10^6 tons. [3] There are several common dehydrogenation methods for the production of styrene monomer from ethylbenzene including adiabatic dehydrogenation of the ethylbenzene, isothermal dehydrogenation of the ethylbenzene, simultaneously producing styrene and oxidation of propylene, membranous process for dehydrogenation of ethylbenzene and dehydrogenation and oxidation of ethylbenzene using carbon dioxide. However, adiabatic dehydrogenation of the ethylbenzene is the most widely used method. Thanks to the recent enhancements in technology, nowadays further developments in the efficiency of the above-mentioned processes have occurred. [5] The main reaction produces styrene and hydrogen.

$$\text{Ethylbenzene} \leftrightarrow \text{styrene} + H_2$$

The dehydrogenation reaction is usually conducted at temperatures above 600°C with an excess of steam. The ethylbenzene dehydrogenation is an endothermic and reversible reaction with an increase in the number of mole due to reaction. High equilibrium conversion can be achieved by a high temperature and a low ethylbenzene partial pressure.[6]

Lowering the boiling point of ethylbenzene allows the use of low level heat to vaporize the ethylbenzene feed to the dehydrogenation reaction system. Despite the use of steam/water to lower the boiling point of ethylbenzene feed, the use of steam reduces the overall energy efficiency of the process. As an alternative, Samsung Total Petrochemicals Co. (Korean Patent Pub. No. 20060092305) used inert gas in place of all or part of the steam to reduce the boiling point of the ethylbenzene feed. However, the addition of inerts to the reactor feed adds to the raw material requirements of the process and the offgas compressor load and power requirements. The inert gas may also not be entirely inert, and may detrimentally affect the equilibrium reaction of ethylbenzene dehydrogenation or the catalyst activity.[7]

A process that economically lowers the boiling point of the ethylbenzene feed in an oxidative ethylbenzene dehydrogenation process has not been reported. As such, there exists an ongoing and unmet need in the industry for economical and energy efficient methods for styrene monomer production from ethylbenzene feedstocks.[7].

Styrene is a building block for the manufacture of a broad range of materials used in thousands of products throughout the world such as rubber, plastic, resins, insulation, fiberglass, pipes, automobile parts, food containers, and carpet backing, due to its strength, flexibility, and lightweight.[7].

Objectives:

- Increasing production of styrene compounds and allied products by using Hysys software version.9.
- Improvement of styrene quality.

II. MATERIALS AND METHODS

A. Description of Process

Ethylbenzene feed is mixed with recycled ethylbenzene, heated and then mixed with high temperature superheated stream . Stream is an inert in the reaction, which is used to drive the equilibrium to ward. Since the formation of styrene is high endothermic , the superheated steam also provides energy to drive the reaction . Decomposition of ethylbenzene to benzene and ethylene , and hydrodealkylation to give methane and toluene are unwanted side reactions . The reactants then enter two adiabatic packed bed reactor (PBR) with inter heating. The products are cooled and it is sent to a three phase separator, in which light gas (H_2, C1 and C_2) , organic liquid , and water exit separate streams. The H_2 stream is farther purified as a source of H_2 else where in the plant. The benzene / toluene stream is currently returned as a feed stream

to the petrochemical facilities. The organic stream containing the desirable product is distilled once to remove benzene and toluene and distilled again to separate unreacted ethylbenzene for recycle the styrene product.

B. Major reaction

$$C_6H_5C_2H_5 \leftrightarrow C_6H_5C_2H_3 + H_2$$
Ethyl Benzene — Styrene — Hydrogen

C. Side reaction

$$C_6H_5C_2H_5 \rightarrow C_6H_6 + C_2H_4$$
Ethyl Benzene — Benzene — Ethylene

$$C_6H_5C_2H_5 \rightarrow 8\,C + 5\,H_2$$
Ethyl Benzene — Carbon — Hydrogene

C. Styrene also reacts catalytically to toluene

$$C_6H_5C_2H_3 + 2H_2 \rightarrow C_6H_5CH_2 + CH_4$$
Ethyl Benzene — Hydrogene — Toluene — Methane

Since styrene is spontaneously polymerized at high temperature, it suggests that temperature of styrene should be maintain at less than 125°C in vacuum condition for a spontaneous reaction.

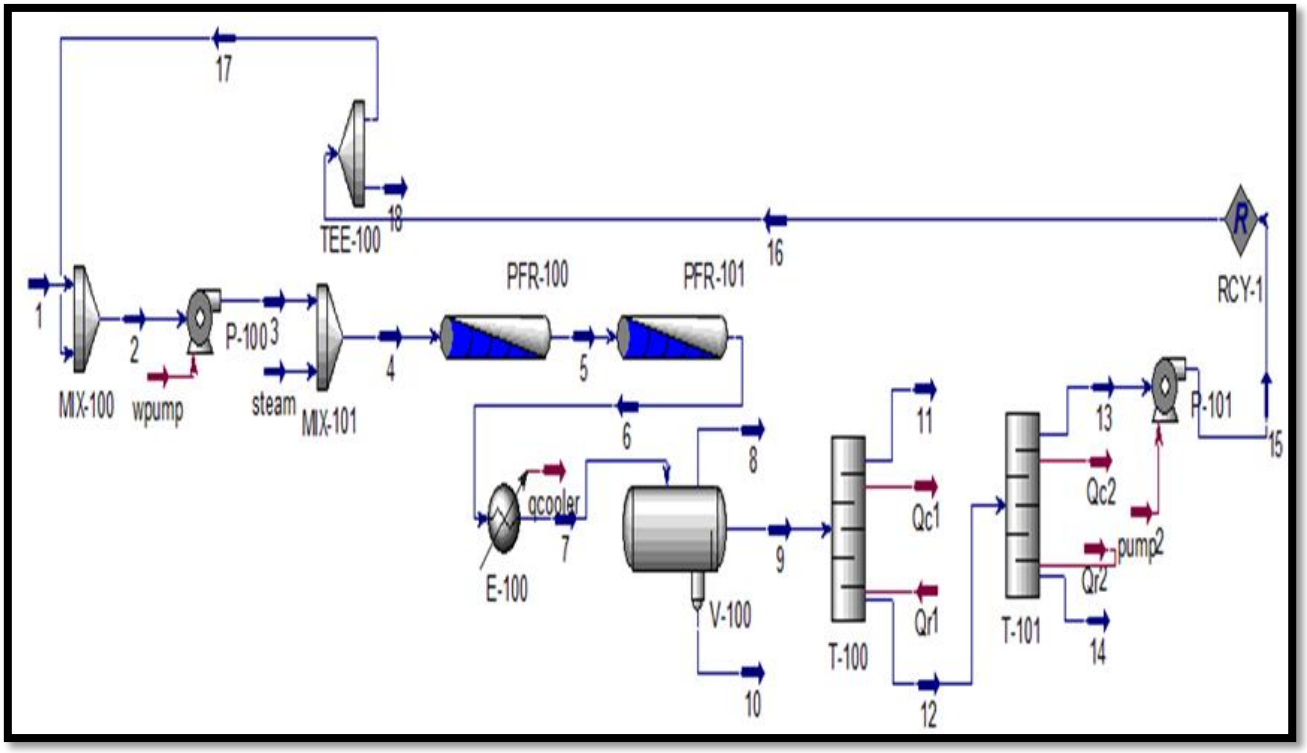

Figure.1: Dehydrogenation a process steady state simulation

Equipment Description

MIX-100	Mixer 1,	P-100	Pump 1,	MIX-101	Mixer 2,	E-100	Cooler,
P FR-100	Plug Flow Reactor 1	V-100	3 Phase Separator,	TEE-100	Tee	P-101	Pump 2
PFR-101	Plug Flow Reactor2,	T-100	Shortcut column 1,	Rey-100	Recycle 1	T-101	Shortcut column 2

Aspen HYSYS:

This Aspen HYSYS simulation models the production of styrene from EB by dehydrogenation: a process using a two-stage reactor with steam reheats. The process consists of three sections: dehydrogenation, vent gas and condensate treatment, and styrene recovery.

III. RESULT AND DISCUSSION

In the following figures, sensitivity analysis was developed for different ranges operating condition (temperature, pressure and flow rate with reactor length. Results for sensitivity analysis are presented in plots:

Figure.2 show the temperature of PFR 100 as a function of reactor length. As expected, the temperature decreases with the length of reactors due to the high endothermic reaction of dehydrogenation of ethylbenzene to styrene.

Figure.3 depicts, pressures vs. the length of reactor R-100, as the pressure distribution within the reactor has decreasing along the reactor. The feed pressure much above than 2 bar, such as 2.5 bar, is not allowed in this simulation because It has been proven the process is favored at low pressure 2.00 bar.

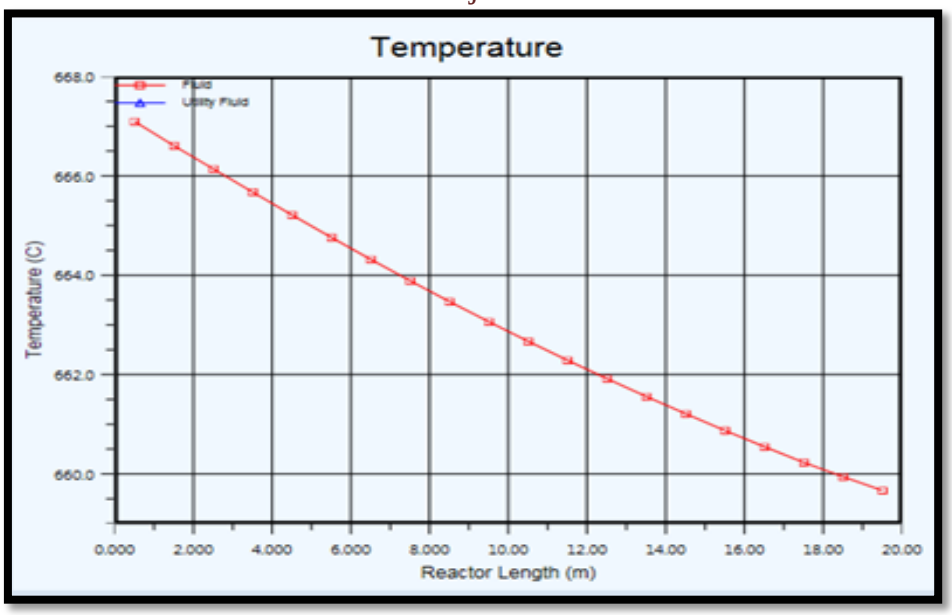

Figure 2: Temperature variation along the PFR100

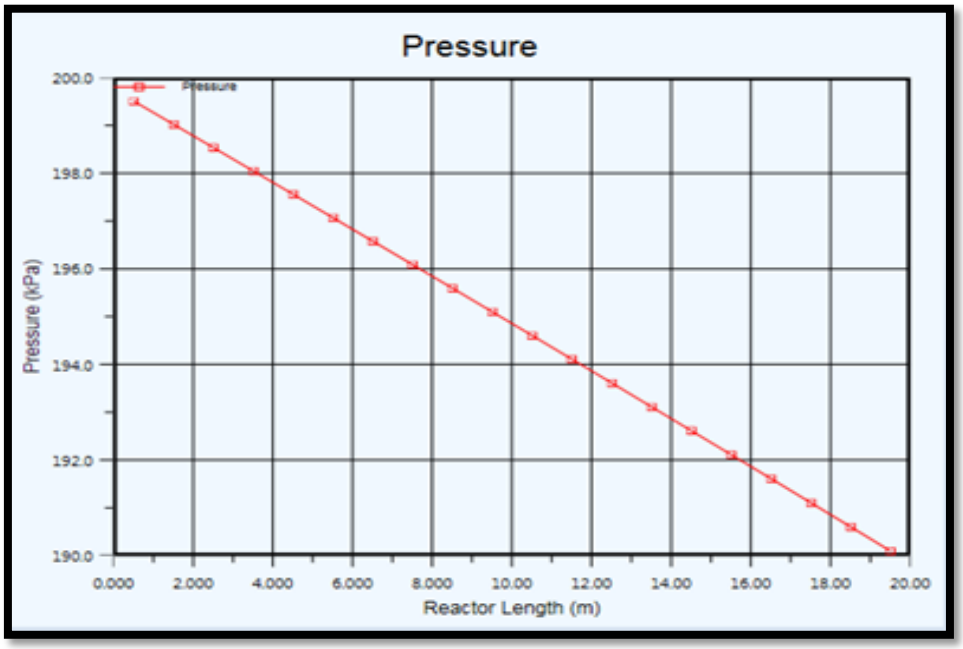

Figure 3: Pressure drop variation along the PFR100.

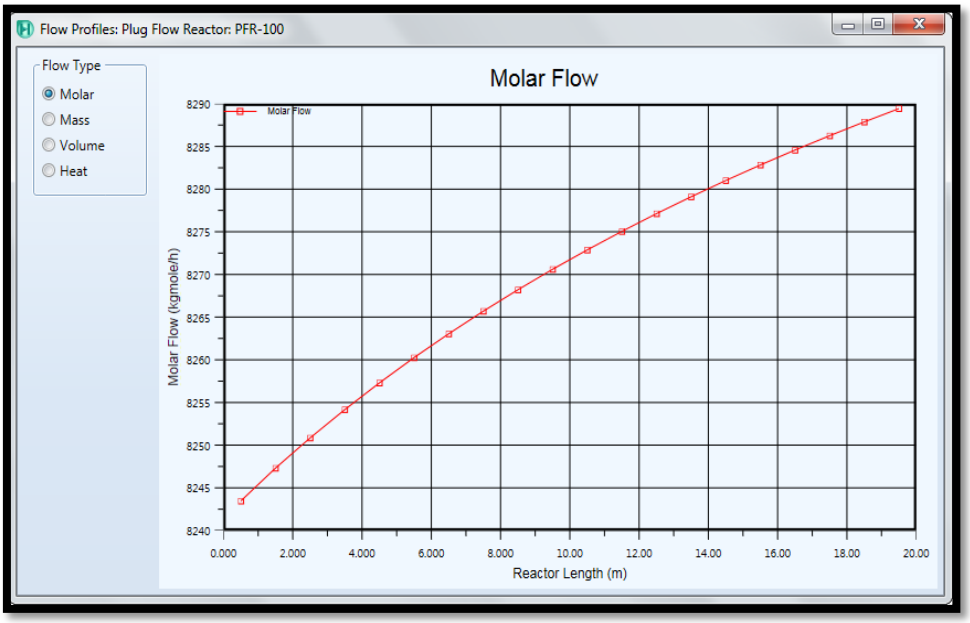

Figure 4: Effect of reactor length on the molar flow in the plug flow reactor.

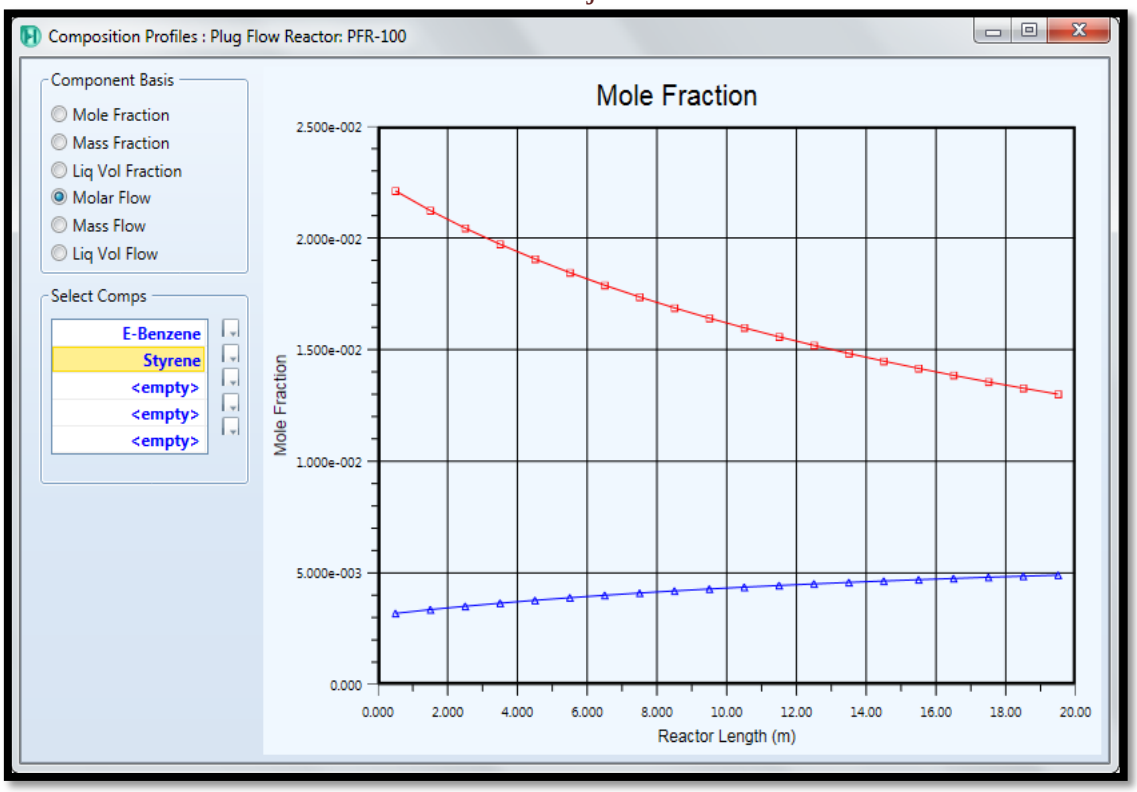

Figure 5: Effect of PFE100 length on the Styrene, EBZ flow rate.

Figure 5 show the behavior of ethylbenzene and styrene's mole fraction vs the length of reactor PFR100 .As Figure.5 shows, ethylbenzene decreases along the reactor; styrene monomer is produced and slope increases.

CONCLUSION

- The dehydrogenation process was simulated by the aspen Hysys software version.9 and it gave goodresults compared with the hand calculation.
- One of the most important results obtained from this work is that it is very important to make sensitivity analysis for the process.
- Form the sensitivity analysis performed ,it can been seen that the optimum inlet temperature 933^{o}K ,which is close to the inlet temperature used in industrial process .It has been proven the process is favored at low pressure 2.00 bar..

Recommendations

From the above, the following improvements are recommended:

- Using Aspen HYSYS program to develop any process will be very helpful because it is very accurate and very helpful in equipment design and selection of the optimum operating conditions.
- Detail studies can be taken for accurate selection of operation conditions and equipment specifications.
- As this unit is a downstream unit, there are many factors which affect it, so it is recommended to make a simulation of all the process in order to accurately indicate the conditions affecting the process.

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References

[1] www. kpatents.com
[2] Product Focus: Styrene. Chemical Week, May 15, 2002, p. 36.
[3] Chemical Profile. Chemical Market Reporter, May 14, 2001, p. 37.
[4] James, D. H.; Castor, W. M. Styrene. In Ullmann's Encyclopedia of Industrial Chemistry; Campbell, F. T.,Pfefferkorn, R.,Rounsaville, J. F., Eds.; Wiley-VCH:
Weinheim, 1994; Vol. A25, p. 329.
[5] Yousef Tamsilian, Ali Nejad Ebrahimi, Ahmad Ramazani S.A., Himan Abdollahzadeh, "Modeling and sensitivity analysis of styrene monomer production process and investigation of catalyst behavior", Computers and Chemical Engineering 1-11, 2012.
[6] Won Jaelee, "Ethylbenzene Dehydrogenation into Styrene, Kinetic Modeling and Reactor Simulation", Department of Chemical Engineering, Texas A&M University , December 2005.
[7] Kevin J. Schwint , Richard J. Wilcox , " Process for the production of styrene monomer by improving energy efficiency and injecting a recycle gas into the EB vaporizer", Lummus Technology Inc. 2011