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Research Article

Improving Yield Conversion with Triple Conversion Reactor for Styrene Production from Ethylbenzene

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Abstract

Styrene is a critical component in various polymer-based materials, with increasing global demand. Its production primarily involves the catalytic dehydrogenation of ethylbenzene, a process requiring high temperatures and facing challenges like by-product formation. This research aims to enhance the yield conversion of styrene using a triple conversion reactor system. The methodology employs Aspen HYSYS simulation, with thermodynamic considerations guiding the reactor designs and operating conditions. Results indicate that implementing three reactors increased the conversion rate from 96% to 99.9% and achieved 99.5% styrene purity. The study concludes that process optimization significantly improves the efficiency and scalability of industrial styrene production.

Keywords: Styrene; Etilbenzene; Dehydrogenation; Process modification; Improving Yield

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1. Introduction

Styrene ($C_6H_5CH{=}CH_2$, phenyl ethylene, vinyl benzene) is the common name given to the simplest and most important member of the unsaturated aromatic monomers family [1]. Styrene is a major component of many polymer-based products so that a steady increasing in worldwide production is expected in the next years [2]. It is used to produce versatile polymeric materials, the main products being poly-styrene, styrene-acrylonitrile, styrene-butadiene latex and acrylonitrile-butadiene styrene resins. The utilization of styrene-based plastics is growing quickly [3]. Currently, polystyrene is the least expensive thermoplastics in terms of a cost-pervolume basis. The major commercial process to produce styrene is the dehydrogenation of ethylbenzene, in which adiabatic dehydrogenation accounts to 90% of the commercial production [4].

Styrene is predominantly produced via direct dehydrogenation of ethylbenzene on an iron-based catalyst. Typically, the conversion rate of ethylbenzene to styrene is around 50–70% per pass across the dehydrogenation reactor. Ethylbenzene is almost exclusively (>99 %) used as an intermediate for the manufacture of styrene monomer, 50 % of the world's benzene production is consumed for this purpose. Less than 1 % of the ethylbenzene produced is used as a paint solvent or as an intermediate for other chemicals [5]. Currently, al most all ethylbenzene is produced commercially by alkylating benzene with ethylene, primarily via two routes: in the liquid phase with aluminum chloride catalyst (Friedel-Crafts reaction), or in the vapor phase with a fixed

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bed of either a Lewis acid or a synthetic zeolite catalyst developed by Mobil Corporation [6].

Many previous studies on styrene production have discussed increasing production or efficiency energy [7]. However, research on yield conversion in styrene production is still limited. Thus, the aim of this research is to increase the conversion yield of styrene production from ethylbenzene by using three conversion reactor units.

2. Method

2.1 Property Package

Aspen HYSYS has completed with various thermodynamic equations. The selection of appropriate equations is aimed at analyzing phase equilibrium and the enthalpy of mixed compounds. In this simulation of the process for styrene production, the Soave-Redlich Kwong (SRK) property package was used.

2.2 Dehydrogenation

The styrene production process used ethyl benzene dehydrogenation, which is the most widely used process in producing styrene on a commercial scale (Figure 1). Dehydrogenation is an endothermic reaction that requires heat for the reaction to occur and high temperatures are required to achieve high conversions [8]. The exothermic reaction during dehydrogenation will become endothermic during the hydrogen addition and the regeneration process [1]. As a result, in addition to the energy constraints on the endothermic reaction for dehydrogenation, energy constraints exist for the exothermic reaction during hydrogenation. With the coupled reactions, the heat from the endothermic reaction could be used during regeneration to support the regeneration of the exothermic reaction [9]. The reaction of styrene formation from dehydrogenation of ethyl benzene as follows.

Reaction 1: styrene formation reaction from ethylbenzene:

$$C_6H_5CH_2CH_3 \rightarrow C_6H_5CH{=}CH_2 + H_2 \quad \Delta H_{r,298K} = 117.57 \text{ kJ/mol} \tag{1}$$

Also there is a side reaction in the form of the formation of benzene and toluene with the reaction can be seen in reactions 2 and 3.

Reaction 2: benzene formation side reaction

$$C_6H_5CH_2CH_3 \rightarrow C_6H_6 + C_2H_4 \quad \Delta H_{r,298K} = 105.4 \text{ kJ/mol} \tag{2}$$

Reaction 3: benzene formation side reaction

$$C_6H_5CH_2CH_3 + H_2 \rightarrow C_6H_5CH_3 + CH_4 \quad \Delta H_{r,298K} = -56.64 \text{ kJ/mol} \tag{3}$$

The dehydrogenation process of ethyl benzene to styrene consists of four stages as follows:

(a) Preparation and mixing of raw materials in the form of ethyl benzene with water vapor: At this stage, ethyl benzene as raw material is prepared at a temperature of 375 °C by looking for heating using a heater. Ethyl benzene which before heated is mixed using a recycle stream that still contains composition of ethyl benzene in the mixer. Further mixing is carried out on ethyl benzene and steam with a mass flow ratio of 1: 3 using a mixer. Output from the mixer will then be used as feed to the reactor.

(b) Dehydrogenation: The dehydrogenation reaction is carried out in the conversion reaction operating endothermically at a temperature of 600 – 630 °C and a pressure of 1,4 atm. At the output of the reactor, styrene has begun to form which still contains other compound compositions. The output of the reactor is then flowed to the cooler to reduce the temperature [10].

(c) Cooler: The reactor output mixture is cooled using a cooler to reaches a temperature of 25 °C. The cooler output is then flowed to the separator to get the styrene component.

(d) Separation: The separation process is carried out to obtain styrene with high purity [11]. In this separation process using 2 distillation columns (conventional distillation). The top result in the first distillation column is returned as recycle because it still contains ethyl benzene as a component [12]. The bottom result in the second distillation column is flowed to the second distillation column to obtain styrene with higher purity.

2.1 Thermodynamics Consideration

Thermodynamic examination is used to determine the nature and direction of reactions, i.e. exothermic / endothermic and reversible/irreversible. In the process in this simulation, three conversion reactors is used. As

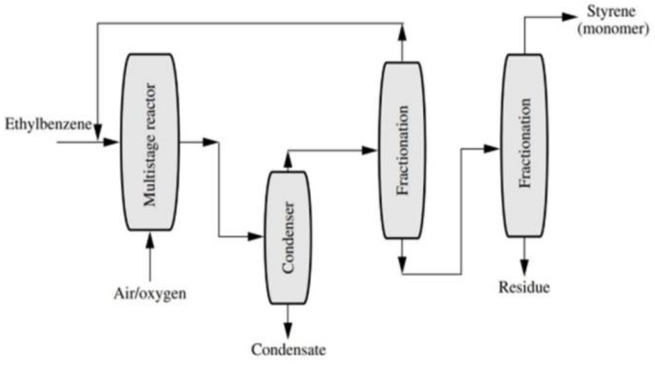

Figure 1. Basic block diagram of styrene process from ethyl benzene [4]

for the main reaction in the reactor, the value of $\Delta H^o_{f,298K}$ of each component and $\Delta H^o_{r,298K}$ at temperature of 298K can be seen in Table 1. Based on the data in Table 1, the $\Delta H^o_{r,298K}$ reaction is obtained as follow:

Reaction 1:
$\Delta H^o_{r,298K}$ = ΔH Product - ΔH Reactan
$= [(\Delta H_{f,\ C_6H_5CH=CH_2} + \Delta H_{f,\ H_2}) - (\Delta H_{f,\ C_6H_5CH_2CH_3})]$
$= [(147.36 + 0) - (29.79)] = 117.57$ kJ/mol
Reaction 2:
$\Delta H^o_{r,298K}$ = ΔH Product - ΔH Reactan
$= [(\Delta H_{f,C6H6} + H_{f,C2H4}) - (H_{f,C6H5CH2CH3})]$
$= [(\Delta H_{f,\ C_6H_6} + \Delta H_{f,\ C_2H_4}) - (\Delta H_{f,\ C_6H_5CH_2CH_3})]$
$= [(82.93 + 52.30) - (29.79)] = 105.4$ kJ/mol
Reaction 3:
$\Delta H^o_{r,298K}$ = ΔH Product - ΔH Reactan
$= [(\Delta H_{f,\ C_6H_5CH_3} + \Delta H_{f,\ CH_4}) - (\Delta H_{f,\ C_6H_5CH_2CH_3})]$
$= [(\Delta H_{f,\ C_6H_5CH_3} + \Delta H_{f,\ CH_4}) - (\Delta H_{f,\ C_6H_5CH_2CH_3} + \Delta H_{f,\ H_2}]$
$= [(147.36 + 0) - (29.79 + 0)] = [(50 + (-74.85) - (29.79 + 0)] = -56.64$ kJ/mol

The value $\Delta G^o_{f,298K}$ of each component at temperature of 298 K can be seen in Table 2. Based on the data in Table 2., the $\Delta G^o_{r,298K}$ of main reaction is obtained as follow:

Reaction 1:
$\Delta G^o_{r,298K}$ = ΔG Product - ΔG Reactan
$= [(\Delta G_{f,\ C_6H_5CH=CH_2} + \Delta G_{f,\ H_2}) - (\Delta G_{f,\ C_6H_5CH_2CH_3})]$
$= [(213.80 + 0) - (130.58)] = 83.22$ kJ/mol
The magnitude of the equilibrium constant (K) at 298 K can be calculated as:
$\ln K_{298} = -\Delta G^o_{r,298K}/RT$
$\ln K_{298} = (-(83220\ \text{J/mol})/(8.314\ \text{J/mol})(298\ \text{K})$
$\ln K_{298} = -33.589$
$K = 2.585 \times 10^{-15}$

At reactor temperature of 700°C (973 K) the magnitude of the equilibrium constant (K) can be calculated as follow:

$\ln K_{298}/K_{973} = -\Delta H/R$
$$\ln \frac{2.585\times10^{-15}}{K973} = \frac{117570\ J/mol}{8.314 \frac{J}{mol}.K}\left[\frac{1}{298} - \frac{1}{973}\right]$$
$K_{973} = 0.512$

Based on the calculations we have done, we get K at 973 K = 0.512 and the reaction occurs reversibly.

Reaction 2:
$\Delta G^o_{r,298K}$ = ΔG Product - ΔG Reactan
$= [(\Delta G_{f,\ C_6H_6} + \Delta G_{f,\ C_2H_4}) - (\Delta G_{f,\ C_6H_5CH_2CH_3})]$
$= [(129.66 + 68.12) - (130.58)]$
$= 67.2$ kJ/mol

The magnitude of the equilibrium constant (K) at 298 K can be calculated as:

$\ln K_{298} = -\Delta G^o_{r,298K}/RT$
$\ln K_{298} = (-(67200\ \text{J/mol})/(8.314\ \text{J/mol})(298\ \text{K})$
$\ln K_{298} = -27.123$
$K = 1.662 \times 10^{-12}$
At reactor temperature of 700 °C (973 K) the magnitude of the equilibrium constant (K) can be calculated as follow:
$\ln K_{298}/K_{973} = -\Delta H/R$
$$\ln \frac{1.662\times10^{-12}}{K973} = \frac{105400\ J/mol}{8.314 \frac{J}{mol}.K}\left[\frac{1}{298} - \frac{1}{973}\right]$$
$K_{973} = 10.907$

Table 1. Entalphy formation of components and entalphy of reaction of the main reaction [13]

Compounds	Molecular Formula	$\Delta H^o_{f,298K}$ (kJ/mol)
Ethylbenzene	$C_6H_5CH_2CH_3$	29.79
Styrene	$C_6H_5CH=CH_2$	147.36
Hydrogen	H_2	0
Benzene	C_6H_6	82.93
Ethylene	C_2H_4	52.30
Toluene	$C_6H_5CH_3$	50
Methane	CH_4	-74.85

Table 2. Gibbs' free energy formation of components on the reactor [13]

Compounds	Molecular Formula	$\Delta G^o_{f,298K}$ (kJ/mol)
Ethylbenzene	$C_6H_5CH_2CH_3$	130.58
Styrene	$C_6H_5CH=CH_2$	213.80
Hydrogen	H_2	0
Benzene	C_6H_6	129.66
Ethylene	C_2H_4	68.12
Toluene	$C_6H_5CH_3$	122.01
Methane	CH_4	-50.84

Based on the calculations we have done, we get K at 973 K = 10.907 and the reaction occurs reversibly.

Reaction 3:
$\Delta G^{o}_{r,298K}$ = ΔG Product - ΔG Reactan
$= [(\Delta G_{f,\ C6H5CH3} + \Delta G_{f,\ CH4}) - (\Delta G_{f,\ C6H5CH2CH3})]$
$= [(\Delta G_{f,\ C6H5CH3} + \Delta G_{f,\ CH4}) - (\Delta G_{f,\ C6H5CH2CH3} + \Delta G_{f,\ H2}]$
= 122.01 + (-50.84) – (130.58 + 0) = -59.41 kJ/mol
The magnitude of the equilibrium constant (K) at 298 K can be calculated as:

$\ln K_{298} = -\Delta G^{o}_{r,298K}/RT$
$\ln K_{298} = (-(-59410\ J/mol)/(8.314\ J/mol)(298\ K)$
$\ln K_{298} = -23.979$
$K = 2.594 \times 10^{10}$

At reactor temperature of 700 °C (973 K) the magnitude of the equilibrium constant (K) can be calculated as follow:

$\ln K_{298}/K_{973} = -\Delta H/R$
$$\ln \frac{2.594\times10^{10}}{K973} = \frac{(-54540)\ J/mol}{8.314\frac{J}{mol}.K}\left[\frac{1}{298} - \frac{1}{973}\right]$$
$K_{973} = 5881.804$

Based on the calculations we have done, we get K at 973 K = 5881.804 and the reaction occur reversibly.

2.4 Method to Improve Yield and Conversion of Styrene Production from Ethylbenzene

The production of styrene from ethylbenzene primarily involves the catalytic dehydrogenation of ethylbenzene, which is an endothermic reaction requiring high temperatures, typically around 600 °C [14]. This reaction not only produces styrene but also generates by-products such as benzene and toluene [15]. To optimize the overall yield of styrene while minimizing these by-products, a multi-reactor system combined with effective cooling and distillation techniques is essential [16].

First Reactor: The initial reactor operates under high temperature and low pressure conditions to maximize the conversion of ethylbenzene to styrene. The reaction conditions are optimized to favor the production of styrene while controlling the formation of by-products [17].

Second Reactor: The effluent from the first reactor, containing unreacted ethylbenzene and various by-products, is fed into a second reactor. This reactor is designed to further convert any remaining ethylbenzene, thus increasing the overall yield of styrene. By maintaining specific temperature and pressure conditions, the reaction can be driven towards higher conversion rates [18].

Third Reactor: The third reactor serves as a polishing step, where any residual ethylbenzene is converted into styrene or other desired products. This step is critical for achieving high purity levels of styrene and maximizing yield conversion [19].

Cooler: The cooling system rapidly reduces the temperature of the effluent, which is crucial for preventing unwanted side reactions, including polymerization of styrene. By controlling the temperature effectively, the cooler ensures that styrene remains in its monomeric form, thereby improving the quality and yield of the final product [20].

3. Result and Discussion

3.1 Comparison of Basic and Modified Process Flow Diagram

The simulation of the process of forming styrene from ethyl benzene process using Aspen HYSYS is depicted in Figures 2 and 4 with respect to basic process and modified process, respectively, while the mass and energy balance is presented in Tabel S1 (Supporting Information). Meanwhile, process flow diagram (PFD) of the basic process and modified process are presented in Figures 3 and 5, respectively. Comparison of styrene yield of basic and modified process is presented in Table 3.

3.2 Process Description of Basic / Unmodified Process

The styrene production process utilizing catalytic dehydrogenation of ethyl benzene was chosen for simulation because it is the most

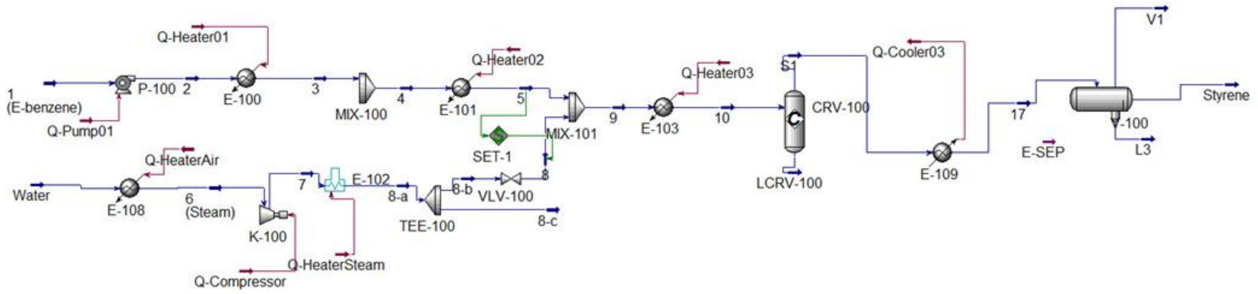

Figure 2. Process simulation of basic process before process creation using ASPEN HYSYS V-11

widely used method in commercial settings for producing styrene [21]. The process involves pre-heating ethyl benzene, mixing and vaporization, dehydrogenation, and subsequent separation/purification. The production begins with a flow of 10,000 kg/h of liquid ethyl benzene, which is pre-heated from ambient temperature (25 °C) to approximately 136 °C using a shell and tube heat exchanger. The pre-heated stream is then mixed with a recycle stream that primarily contains ethyl benzene and water, along with minor amounts of styrene and toluene, sourced from the top of Distillation Column No. 2 (Styrene Column) in a cylindrical pressurized vessel known as the Streams Mixer, which operates under isobaric conditions. The exit stream from the Streams Mixer is fully vaporized in another shell and tube heat exchanger until it reaches around 250 °C. The resulting vapors are directed to another pressurized vessel, also functioning under isobaric conditions (Steam Mixer), where superheated steam is injected to elevate the temperature of the vapor mixture to the reaction condition of 600 °C. The quantity of superheated steam used in the Steam Mixer must be sufficient to achieve a final water/ethyl benzene molar ratio

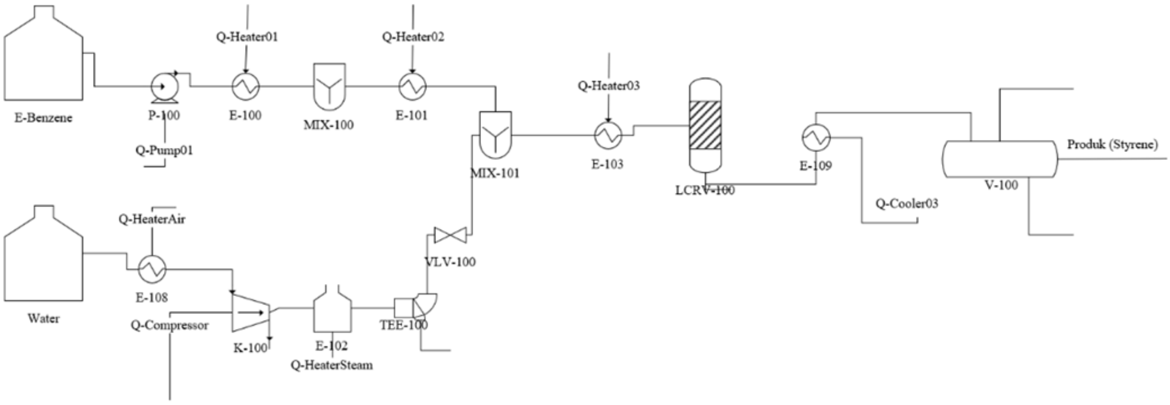

Figure 3. Process Flow Diagram (PFD) of basic process before process creation

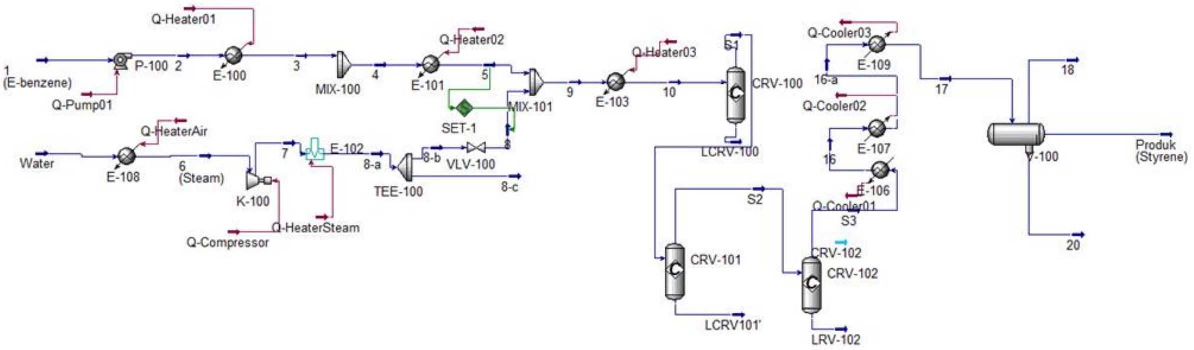

Figure 4. Process simulation of modified process after process creation using ASPEN HYSYS V-11

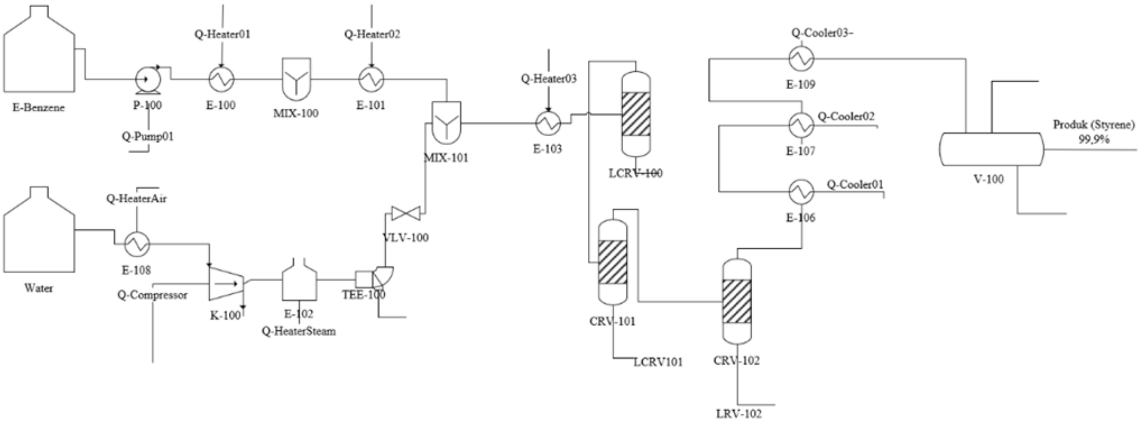

Figure 5. Process Flow Diagram (PFD) of the modified process after process creation

of approximately 14:1 before it is fed into the Conversion Reactor.

The dehydrogenation of ethyl benzene occurs in a reactor that operates isothermally [22]. In this reactor, the gaseous mixture flows superheated steam is injected into the reactor's shell to maintain the reaction temperature within the desired range of 580 to 610 °C. It is crucial to keep the temperature below 610 °C to prevent thermal decomposition of both ethyl benzene and styrene. The exit from the reactor yields a hot gaseous mixture with a styrene mass composition of approximately 93% (on a dry basis). To separate and purify the styrene from other chemicals present in the exit stream (such as water and toluene), the two-phase stream from the coolers is directed to a three-phase separator (Liquid-Liquid-Vapor Separator or LLV Separator), operating at 5 bar and 50 °C. The top of the LLV Separator produces a gaseous mixture primarily composed of hydrogen, methane, and ethylene, along with small amounts of water and styrene (light gaseous stream). Meanwhile, a liquid stream containing water and trace amounts of styrene, benzene, and ethylene is collected at the bottom (wastewater stream). The middle stream (useful stream) mainly consists of styrene with minor quantities of other chemicals and is sent to Distillation Column No. 1 (Benzene-Toluene Column) for recovering benzene and toluene as well as concentrating styrene. Benzene and toluene are collected at the top of Distillation Column No. 1, while a styrene-rich stream is obtained at the bottom and forwarded to Distillation Column No. 2 (Styrene Column) for final purification. In the Styrene Column, styrene is recovered at the bottom with a purity of about 99.5%, while the top stream, which mainly contains ethyl benzene, benzene, and toluene, is recycled back into the process (Recycle Stream) and mixed with pure ethyl benzene that was pre-heated in the initial shell and tube heat exchanger. To prevent spontaneous polymerization of pure styrene at high temperatures and pressures (typically above 6 bar and 125 °C), it is essential to conduct the distillation process at the lowest feasible pressure [23]. This precaution also helps avoid polymerization of vinyl aromatic compounds generated during the reaction phase; thus, the Benzene-Toluene Column operates at a pressure of 1.5 bars, while the secondary distillation in the Styrene Column occurs at atmospheric pressure (1.0 bar) [24].

Table 3. Comparison of styrene yield of basic and modified process

Process	Styrene Yield (%)
Without modification	96
With modification	98.36

3.3 Effect of Process Modification

Modifications to the dehydrogenation process of ethyl benzene to styrene were carried out to optimize the process. Modifications were carried out using three conversion reactors (Table 4). When using one reactor, the resulting conversion only reaches 96%. Meanwhile, when using 3 reactors, the resulting conversion can reach 99.9%. This can be known using the following equation:

$$\text{Conversion (\%)} = \frac{Reacting\ ethyl\ benzene}{Incoming\ ethyl\ benzene}\text{x } 100\% \qquad (4)$$

Ethylbenzene is introduced into a pump at a temperature of 25 ^{o}C and a pressure of 150 kPa. After being pumped, the pressure of ethylbenzene rises to 200 kPa, resulting in product 2. Product 2 is then placed into a heater at a temperature of 25 ^{o}C and a pressure of 200 kPa. After heating, the temperature of ethylbenzene increases to 136 ^{o}C ius, resulting in product 3. Next, ethylbenzene is mixed in a mixer to achieve a more homogeneous solution, and then it is placed into a heater until it reaches a temperature of 250 ^{o}C, resulting in

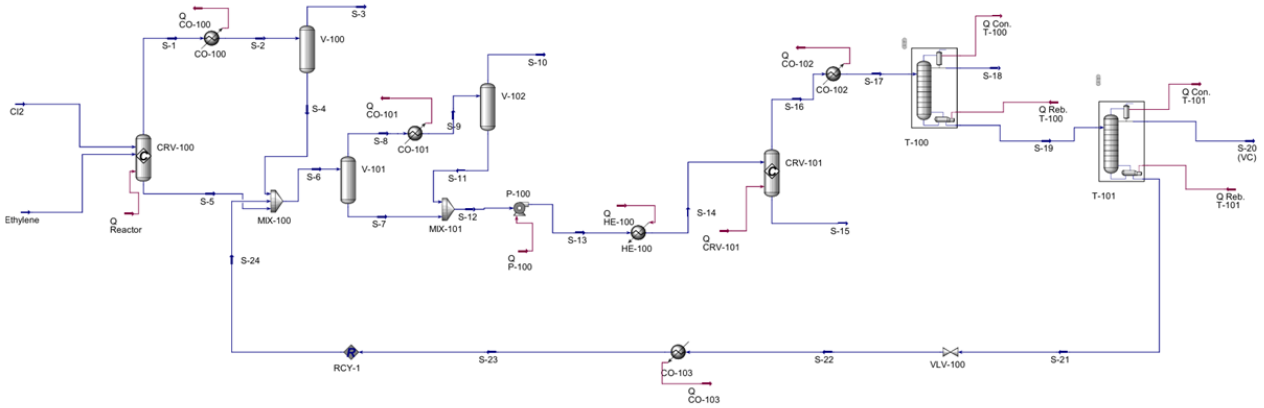

Figure 5. Modified process flow diagram HYSYS Simulation

product 5 [25]. Ethylbenzene is then mixed with steam, which has been heated to 770 °C. This mixture is introduced into a heater at a temperature of 600 °C and subsequently increases to 650 °C, resulting in product 10. The mixture is then fed into a conversion reactor to achieve high purity [26]. In the first conversion reactor, a styrene fraction of 0.066 is produced; in the second conversion reactor, a styrene fraction of 0.067 is produced; and in the final conversion reactor, a styrene fraction of 0.23 is produced. The styrene solution is then passed through a cooler to reduce its temperature from 496.8 °C to 350 °C. The styrene solution continues through the cooler until its temperature reaches 100 °C. Finally, the styrene solution is cooled down to 30 °C us before being introduced into a three-phase separator to separate it from ethylbenzene and water, achieving styrene with a composition fraction of 0.9836.

4. Conclusions

This study demonstrates the optimization of styrene production from ethylbenzene through process modification using Aspen HYSYS simulation. Using a three-reactor system, the conversion efficiency increased from 96% to 99.9%, demonstrating the effectiveness of multi-stage catalytic dehydrogenation. Key process improvements included precise control of reaction conditions - such as temperature, pressure, and molar ratio to maximize styrene yield while minimizing byproducts such as benzene and toluene. Advanced cooling and separation techniques further ensure high-purity (99.5%) styrene yields and reduced energy consumption. These improvements underscore the potential of this method to increase efficiency and scalability in industrial styrene production.

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Table 4. Data performance of reactor in the modified process

Parameter	Reactor 1	Reactor 2	Reactor 3
Temperature in (°C)	650	508.5	508.5
Temperature out (°C)	508.5	508.5	507.1
Molar Flow in (kgmole/h)	745.6	794.7	794.7
Molar Flow out (kgmole/h)	794.7	794.7	795.2
E-benzene	0.0006	0.0006	-
Styrene	0.0653	0.0653	0.0659
Hydrogen	0.0618	0.0618	0.0623
Toluene	0.0010	0.0010	0.0010
H_2O	0.8713	0.8713	0.8708

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