Production of Ethylbenzene by Liquid Phase Reaction

CHE251

Date of Submission: 10/11/2024

Group 4

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Modeling an Efficient and Robust Ethylbenzene Production System in ASPEN

Abstract

This report presents the simulation and optimization of an ethylbenzene (EB) production system using ASPEN. The focus is on maximizing ethylbenzene yield, minimizing by-product formation, and designing an efficient system with optimized reactor parameters and recycle flows. The process is analyzed using reaction kinetics, thermodynamic models, and energy consumption assessment.

1 Introduction

Ethylbenzene (EB) production is a crucial process in the petrochemical industry. The process involves the liquid-phase reaction between ethylene (C_2H_4) and benzene (C_6H_6) to produce ethylbenzene. The main objectives of this study are to maximize the yield of ethylbenzene, minimize by-products like di-ethylbenzene (DEB), and optimize the reactor and separation processes using ASPEN simulation.

2 Objective

The primary goals of the study are:

- Maximize the yield of ethylbenzene.
- Minimize the formation and accumulation of byproducts.
- Optimize reactor parameters and recycle flows for improved performance.
- Focus on precise temperature, pressure, and composition control to maintain high selectivity and conversion.
- Study the liquid-phase reaction between ethylene and benzene to produce ethylbenzene in a continuous stirred-tank reactor

3 Flow Sheet / Block Diagram

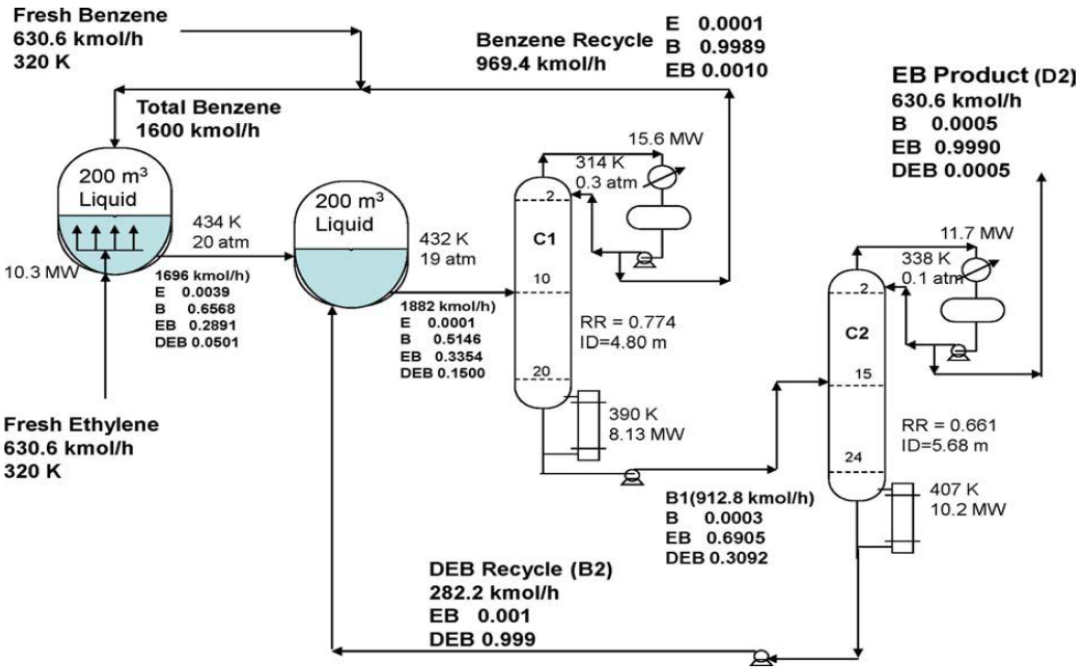

Figure 1: Process Flow Diagram for Benzene and Ethylene Reaction System

4 Methodology

4.1 Feed Preparation

The feed preparation includes the purification of benzene and ethylene to remove impurities, followed by compression and heating to achieve optimal reaction conditions for the reactor.

4.2 Reaction Kinetics

The production of ethylbenzene follows the liquid-phase reaction between ethylene and benzene, represented as:

$$C_2H_4 + C_6H_6 \rightarrow C_8H_{10} \tag{1}$$

However, there are undesirable side reactions:

$$C_8H_{10} + C_2H_4 \rightarrow C_{10}H_{14} \quad \text{(Formation of Di-Ethylbenzene)} \tag{2}$$

In addition, a third reaction occurs where DEB reacts with benzene to regenerate ethylbenzene:

$$C_{10}H_{14} + C_6H_6 \rightarrow 2C_8H_{10} \tag{3}$$

This reaction allows for the recycling of DEB back into the system, where excess benzene drives the reaction to produce more ethylbenzene, effectively reducing DEB accumulation.

The reaction kinetics are summarized in Table 1.

Table 1: Reaction Kinetics and Activation Energy

Reaction	**Rate Constant (k)**	**Activation Energy (E) (cal/mol)**
$C_2H_4 + C_6H_6 \rightarrow C_8H_{10}$	1.528×10^6	17,000
$C_8H_{10} + C_2H_4 \rightarrow C_{10}H_{14}$	2.778×10^7	20,000
$C_{10}H_{14} + C_6H_6 \rightarrow 2C_8H_{10}$	1000	15,000

As the activation energy for the formation of di-ethylbenzene (Reaction 2) is larger than that for the desired ethylbenzene formation (Reaction 1), it is essential to maintain lower reactor temperatures to improve selectivity. Additionally, maintaining a large excess of benzene helps reduce the concentrations of ethylene and ethylbenzene, which further enhances selectivity.

5 Energy Consumption and Generation of Components

Table 2: Energy Consumption and Generation in Components

Components	**Energies (kW)**
COMP	2482
PUMP1	107
PUMP2	3
PUMP3	39
Heat Exchanger	-1537
CSTR1	-11348
DISTILL1 (QC)	-16387
DISTILL2 (QC)	-13576
DISTILL2 (QR)	9438
DISTILL2 (QR)	11010

5.1 Separation and Recycle

After the reaction, the reactor effluent is cooled, and a distillation column is used to separate unreacted reactants from heavier products. Further distillation isolates ethylbenzene from di-ethylbenzene and other higher molecular weight compounds. Unreacted ethylene and benzene are recycled back to the reactor. Di-ethylbenzene (DEB) can be sent to a hydrocracking unit for recovery of valuable components.

5.2 ASPEN Simulation Setup

- **Thermodynamic Properties:** The Peng-Robinson equation of state is used for property calculations.
- **Reactor Modeling:** A convergent reactor system models the reaction process, ensuring precise control over temperature and pressure.
- **Distillation Modeling:** A rigorous stage-by-stage method is used for the distillation columns to ensure efficient separation.

6 Results and Discussion

6.1 Process Performance

The impact of various operating conditions on the conversion, selectivity, and yield was analyzed. Factors such as temperature, pressure, and feed composition were studied to identify optimal conditions for maximizing ethylbenzene production and minimizing byproduct formation.

6.2 Energy Consumption

The energy consumption for each major unit operation is summarized in Table 3, which includes compression, heating, reactor operation, and distillation.

Table 3: Energy Consumption per Process Step

Process Step	**Energy Consumption (kWh)**	**Description**
Compression	10	Compression of feed mixture
Heating	8	Heating to reaction temperature
Distillation	15	Separation of products and unreacted feed
Reactor Operation	12	Operation of CSTR

7 Conclusion

The ASPEN simulation of the ethylbenzene production process revealed that optimal temperature, pressure, and feed composition are essential for maximizing ethylbenzene yield and minimizing byproducts. The recycling of DEB back into the reactor is effective in reducing waste and enhancing EB production. Energy consumption analysis shows that distillation and reactor operation are the most energy-intensive steps, and improvements in these areas could lead to significant energy savings.

8 Data Table Image

	Units	DIETHBEN	BOTFEED	DIETHBEN	ETHBENZ	ETHYLENE	BENZENE	RECYCBZ	RECYCDB	S1
Description										
From		DISTILL2	DISTILL1	DISTILL2	DISTILL2			PUMP2	PUMP3	MIX1
To		PUMP3	DISTILL2	PUMP3		COMP	MIX1	MIX1	MIX3	PUMP1
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
MIXED Substream										
Phase		Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase	Vapor Phase	Liquid Phase	Liquid Phase	Liquid Phase	Liquid Phase
Temperature	C	168.7905239	145.0073771	168.7905239	64.62621839	46.85	320	42.0497747	169.9926834	43.94242427
Pressure	atm	0.9997532692	0.9997532692	0.9997532692	0.09997532692	1	1	0.9997532692	18.89958056	0.9997532692
Mole Flows	kmol/hr	282.2	912.8	282.2	630.6	630.6	630.6	969.4	282.2	1600
Mole Fractions										
BENZE-01		2.96E-14	0.000457680458	2.96E-14	0.000662497181	0	1	0.9899999544	2.96E-14	0.9939412667
ETHYL-01		0	7.86E-34	0	0	1	0	7.47E-05	0	4.53E-05
EB		0.2365483302	0.7630570442	0.2365483302	0.9986751204	0	0	0.009925345968	0.2365483302	0.00601347462
DEB		0.7634516698	0.2364852753	0.7634516698	0.000662382444	0	0	6.81E-09	0.7634516698	4.13E-09
Mass Flows	kg/hr	36004.51237	102953.6728	36004.51237	66949.16041	17690.70106	49258.46138	75989.6612	36004.51237	125248.1206

Figure 2: Process data table from spreadsheet

	Units	S2	S3	S4	S5	S6	S7	S8	S9	TOPBENZ
Description										
From		PUMP1	COMP	COOLER	MIX2	CSTR1	MIX3	CSTR2	VALVE	DISTILL1
To		MIX2	COOLER	MIX2	CSTR1	MIX3	CSTR2	VALVE	DISTILL1	PUMP2
Stream Class		CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN	CONVEN
MIXED Substream										
Phase		Liquid Phase	Vapor Phase	Vapor Phase		Liquid Phase	Liquid Phase	Liquid Phase		Liquid Phase
Temperature	C	44.9371202	297.8555615	160.9	63.00424938	160.9	163.1503136	166.4741963	122.6192991	42.00887155
Pressure	atm	20	20	19.89637306	19.89637306	18.89958056	18.89958056	17.90278806	1.500123365	0.3000246731
Mole Flows	kmol/hr	1600	630.6	630.6	2230.6	1606.179312	1888.379312	1882.2	1882.2	969.4
Mole Fractions										
BENZE-01		0.9939412667	0	0	0.712949891	0.65232716	0.5548431834	0.5101071759	0.5101071759	0.9899999544
ETHYL-01		4.53E-05	1	1	0.282736666	0.003892291954	0.003310626616	3.85E-05	3.85E-05	7.47E-05
EB		0.00601347462	0	0	0.004313440057	0.2928092422	0.2844015946	0.3751674107	0.3751674107	0.009925345968
DEB		4.13E-09	0	0	2.96E-09	0.05097130586	0.1574445954	0.114686944	0.114686944	6.81E-09
Mass Flows	kg/hr	125248.1206	17690.70106	17690.70106	142938.8216	142938.8216	178943.334	178943.334	178943.334	75989.6612

Figure 3: Process data table from spreadsheet

9 References

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