



## Intensification of the ethylbenzene production process using a column configured with a side reactor

Arif Hussain, Le Quang Minh, Moonyong Lee\*

Process System Design & Control Laboratory, School of Chemical Engineering, Yeungnam University, Dae-Dong 214-1, Gyeongsan, 712-749, South Korea



### ARTICLE INFO

#### Keywords:

Side-reactor distillation  
Ethylbenzene production  
Heat integration  
Energy savings  
Process intensification

### ABSTRACT

An innovative heat-integrated column configured with a side-reactor was developed for ethylbenzene (EB) production. To achieve an economical design, the total annual cost, as an objective function, was minimized by optimizing the reactor volume, the number of side reactors, the number of column trays, the reactor side-return tray, and the column pressure. The proposed side-reactor column (SRC) configuration reduces capital, energy, and total annual costs by 13.6, 12.9, and 13.2%, respectively, compared to a conventional process for the same desired yield and purity. In addition, the multiple effect heat integration was examined on the proposed configuration for energy efficiency. The resulting heat-integrated side reactor (HI-SRC) configuration further reduces capital, energy, and total annual costs by 14.8, 53.0, and 38.3%, respectively.

### 1. Introduction

Ethylbenzene (EB) is an important commodity chemical that is in high-volume manufacturing demand in the petrochemical industry [1]. Its major use (> 95%) is as an intermediate for the production of styrene [2]. The reaction mechanism involved in the production of EB is a typical example of a multiple-step system, and the economic success of a chemical plant that involves multiple reactions depends on the ability to maximize the formation of the desired product while minimizing the overall energy input [3]. The conventional process for the production of EB features high-pressure reactors followed by downstream low-pressure separation columns. High purity EB is achieved by maintaining a large reactor volume or by using an excess of benzene [4]. Both the former and latter strategies result in high capital and energy costs. However, this classical configuration allows the optimum temperatures for the reactor and distillation to be set independently. The development of an energy efficient and cost-effective production scheme that meets the high-volume market demand for EB is needed. Process-intensified configurations can bring enormous benefits to existing chemical processes by reducing the number of energy-demanding operating units. Reactive distillation (RD) is an excellent example of process intensification; RD integrates the reactor and the separation units into one shell [5,6]. However, RD is economically unattractive when there is a temperature mismatch [7–9]. A side-reactor column (SRC) configuration is an alternative design that overcomes this incompatibility [10]. The SRC is an integrated configuration for reactive distillation processes where the reactors are connected to the column in

an external loop. The side-reactor feed is withdrawn from the column tray where the reactants are abundant and the reactor effluent is returned to the same column. This integrated SRC configuration provides the ability to adjust the column pressure to achieve the desired separation, while the reactor pressure and temperature can be set for the formation of the desired products. Moreover, compared to an integrated multifunctional reactor, the SRC has additional benefits that mainly arise from easier catalyst replacement, easier maintenance, the ability to separately adjust column and reactor pressures and temperatures, and catalysts that do not need to be embedded in complex structures [10].

Few literature studies deal with the design of columns configured with external side reactors. Baur and Krishna [11] proposed a side-reactor design as an alternative to a RD column for methyl acetate synthesis and showed that a higher conversion target requires a larger side-reactor to pump-around ratio in order to match the performance of a RD column. Kaymak and Luyben [12] studied the SRC configuration of a single reversible ideal liquid-phase reaction and showed that the capital and energy costs were significantly lower when a temperature mismatch existed. In an extension of their previous work, Kaymak and Luyben [13] provided a more rigorous steady-state economic optimization of the SRC configuration and went on to further extend their research to the study of the dynamic controllability of the same process and the performance of two different control structures [14]. Cuimei et al. [15] optimized the SRC configuration for chlorobenzene production and proposed an effective control structure for disturbances in production rate and fresh-feed composition. Kolah et al. [16]

\* Corresponding author at: School of Chemical Engineering, Yeungnam University, Gyeongsan, Dae-dong 214-1, South Korea.  
E-mail address: [mynlee@yu.ac.kr](mailto:mynlee@yu.ac.kr) (M. Lee).

introduced a heat-integrated reactive distillation design for triethyl citrate production that used a pre-reactor as well as a side-reactor, and obtained a 98% conversion of citric acid using multiple side-reactors.

The full potential of the side-reactor column (SRC) configuration design is yet to be explored for different chemical processes involving multiple reactions, and where a mismatch between the reactor and distillation operating parameters exists. This paper presents the potential benefits of the SRC design for achieving a given yield and purity of EB in a process that involves multiple reaction steps. The process using the proposed configuration is compared to the conventional (base case) process for the preparation of EB that uses two reactors operated at high pressure followed by two distillation columns operated at low pressure. For the proposed SRC configuration, the total annual cost, as an objective function, was minimized by optimizing the number of side reactors, the number of column trays, the reactor side-return tray, and the column pressure. Moreover, an effective heat integration scheme was developed for the proposed configuration that further saves energy and associated costs.

## 2. The studied process

The production of ethylbenzene (EB,  $C_8H_{10}$ ) was process intensified using the SRC configuration. The irreversible liquid-phase reaction mechanism for the formation of EB is a typical example of a series-type multiple-step process. The first reaction (Eq. (1)) occurs between ethylene (E,  $C_2H_4$ ) and benzene (B,  $C_6H_6$ ) to form ethylbenzene (EB,  $C_8H_{10}$ ). In the second reaction (Eq. (2)), the unreacted ethylene (E,  $C_2H_4$ ) further reacts with ethylbenzene (EB,  $C_8H_{10}$ ) to form diethylbenzene (DEB,  $C_{10}H_{14}$ ). The diethylbenzene (DEB,  $C_{10}H_{14}$ ) also reacts with benzene (B,  $C_6H_6$ ) to reproduce ethylbenzene (EB,  $C_8H_{10}$ ) in a third reaction (Eq. (3)).



The associated kinetic information is summarized in Table 1 and is taken from the work of Luyben [4].

A flowsheet for the conventional production of ethylbenzene, taken from the work of Luyben, is provided for comparison (Fig. 1) [4]. The optimized conventional process uses two continuous stirred-tank reactors connected in series for maximizing ethylene conversion, followed by two distillation columns with two recycle streams for improving the selectivity of the desired product. The yield of ethylbenzene is increased by either increasing the reactor volume or by maintaining a high recycled-benzene flow rate. The resulting process requires high energy and is costly, especially when higher selectivity's are required. Reactive distillation is not a wise choice as reactors are operated at high pressures and temperatures, while the column is operated under vacuum. The application of an SRC configuration could deliver benefits in terms of the low energy required to achieve the desired separation by using the heat of reaction to partially vaporize the product, thereby reducing the reboiler load.

## 3. Proposed configuration

The newly proposed SRC configuration is shown in Fig. 2. All unit

**Table 1**  
Reaction kinetics for the production of ethylbenzene [4].

	Rxn (1)	Rxn (2)	Rxn (3)
Pre-exponential factor	$1.528 \times 10^6$	$2.778 \times 10^7$	1000
E-(cal/mol)	17000	20000	15000
Concentration (kmol/m <sup>3</sup> )	$C_E C_B$	$C_E C_{EB}$	$C_B C_{DEB}$

operations were simulated using Aspen Plus<sup>®</sup>. The semi-empirical Chao-Seader thermodynamic model, as suggested by Luyben, was used in the simulation. [2]

The column C1 is integrated with two external adiabatic tubular reactors. For reactions carried out adiabatically, tubular reactors require smaller volumes than those required by continuous stirred-tank reactors [3]. C1 has a total of 40 stages including the condenser and the reboiler. The stages are numbered from top to bottom. A fresh benzene feed of 630.6 kmol/h, together with recycled benzene from the top of C1, provides a total feed of 1600 kmol/h, which is introduced at stage 12. The less-volatile DEB from the bottom of column C2 is introduced at stage 6. The column operates at 4 atm. The total flow of fresh ethylene feedstock (630.6 kmol/h) is split into two streams and distributed equally into the side reactors. Liquid streams at 941.1 kmol/h from stage 12 (419.7 K) and from stage 14 (454.1 K) are withdrawn and pumped into the external side-reactors R1 and R2, respectively. The volume of each reactor is 90.8 m<sup>3</sup> with an aspect ratio of 5. Reactions occur in the liquid phases inside the high-pressure (20 atm) adiabatic tubular reactors R1 and R2. The high-temperature liquid product streams resulting from the exothermic heats of reaction from reactors R1 and R2 are fed back to column C1 at stages 17 and 19, respectively. The distillate from C1, which is mostly excess benzene, is recycled and fed back to column C1 together with fresh benzene. The bottom produces the desired ethylbenzene together with the diethylbenzene by-product and trace amounts of benzene. The liquid at the bottom of column C1 is fed to stage 15 of a 25-stage column (C2), which separates EB from DEB to 99.9 mol% purity; C2 operates at 0.1 atm. The distillate is the desired ethylbenzene (EB), while the bottom of C2 contains the DEB byproduct that is recycled back to stage 6 of C1.

## 4. Design and optimization of the side-reactor configuration

To avoid an infeasible design, the effects of various design parameters on SRC performance were evaluated using a systematic sequential approach. The total annual cost, as an objective function, was minimized through optimization of the reactor volume, the number of side-reactors, the number of trays, the side-return tray, and the column pressure. The following assumptions were made when designing the proposed SRC configuration.

1. The reactors are of equal size.
2. The tubular side-reactors are adiabatic.
3. The reactor aspect ratio is 5.
4. The kinetically controlled reaction occurs in the liquid phase.
5. The flow rates of the side streams to the side-reactors are equal.

### 4.1. Side-reactor configuration

It is essential to maintain low ethylene concentrations inside the adiabatic tubular reactors to avoid the side reaction that produces DEB and to achieve better selectivity toward the desired product (EB). Ethylene was almost completely converted with excess benzene and was independent of the volume of the side-reactor. Since the excess benzene must be recycled, the approach adopted in this study involved the design and optimization of the side-reactor volumes in order to maximize benzene conversion. Maximizing benzene conversion also helps to reduce the reboiler load of column C1, since lower amounts of benzene that require evaporation and overhead recycling from column C1, will remain. These points are illustrated in Fig. 3a and b for a two-side-reactor system.

Benzene conversion was fixed at 99% in the final reactor connected to the lower stages near the reboiler; the reactors were assumed to be of equal size, with aspect ratios of 5 [17]. Benzene conversion of 99% cannot be achieved in all of the connected side-reactors due to equal size reactors. Initially, one side-reactor was chosen and the volume of the reaction vessel was optimized to achieve this design specification.

Download English Version:

<https://daneshyari.com/en/article/7089428>

Download Persian Version:

<https://daneshyari.com/article/7089428>

[Daneshyari.com](https://daneshyari.com)