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Design and analysis of an ethyl benzene production process using conventional distillation columns and dividing-wall column for multiple objectives

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ABSTRACT

Downstream separation in the ethyl benzene (EB) production is energy intensive due to the use of multiple distillation columns. One technology to achieve significant energy and capital cost savings for this separation, is the use of dividing-wall column (DWC) to replace conventional columns. In the present study, a typical industrial EB process including reaction, separation and heat exchangers, is first simulated rigorously and modified to improve the efficiency and performance of both individual units and the overall plant. DWC is integrated into the EB process, and its performance is compared with the base case of utilizing only conventional columns for downstream separation. All simulations are performed using Aspen HYSYS, and design data used is appropriately validated for realistic simulation. Subsequently, sensitivity analysis is performed on both EB designs for a number of design variables. Objectives selected for sensitivity analysis are net present value, total capital investment and benzene loss. Results show that integrating DWC is not only viable but also offers potential to reduce capital investment, decrease benzene loss and increase profit compared to a conventional column design for the EB process.

1. Introduction

Production of ethyl benzene (EB) is vital due to the importance of products that can be derived from it. Over 90% of EB is utilized to produce styrene monomer, of which 65% is to produce polystyrene, and the remaining is to produce other polymers/copolymers (Gerzeliev et al., 2011). These polymers/copolymers have a large range of applications (Collins and Richey, 1992). Historically, there have been both catalyst upgrades and process modifications for EB production. The previous use of mineral acids such as aluminium chloride is now replaced by zeolite-based catalysts, which offer improved EB selectivity (Ebrahimi et al., 2011), a more environmentally friendly option (Odedairo and Al-Khattaf, 2010) and reduced equipment corrosion (Gerzeliev et al., 2011). Both vapour and liquid-phase alkylation have used zeolite catalysts. Although vapour-phase alkylation represents nearly 50% of EB market globally, it is declining (Netzer and Ghalayini, 2002), primarily due to extreme operating conditions resulting in catalyst deactivation and product contamination (Welch et al., 2005). Hence, the latest trend is towards liquid-phase alkylation using zeolite catalysts, which represents around 23% of the market globally and is increasing worldwide (Netzer and Ghalayini, 2002), offering better catalyst life and optimal thermal control (Perego and Ingallina, 2002). Commercial technologies of liquid-phase zeolite-based alkylation processes include the Lummus/UOP EBOne^{TM} and the Mobil/Badger EBMax^{TM}, which allow for high catalyst stability and relatively low benzene recycle rates. Additional details and benefits of these processes are elaborated in Woodle (2006) and Welch et al. (2005). In 1994, CDTech introduced a mixed liquid-vapour phase alkylation process with zeolite catalyst, utilizing reactive distillation (RD). Although it represents only 2% of the market globally, it is rapidly increasing (Netzer and Ghalayini, 2002). Further, Qi and Zhang (2004) pointed that RD is still in the developmental phase for EB production. Dow Chemical and Indian Petrochemicals Corporation

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Nomenclature

Acronyms

B	Benzene
CDC	Conventional distillation column
CEPCI	Chemical engineering plant cost index
CSTR	Continuous stirred tank reactor
DEB	Di-ethyl benzene
DWC	Dividing-wall column
DV	Decision variable
E	Ethylene
EB	Ethyl benzene
PEB	Poly-ethyl benzene
PF	Pre-fractionator
PFR	Plug flow reactor
PR	Peng–Robinson
RD	Reactive distillation
SRK	Soave–Redlich–Kwong
VLE	Vapour–liquid equilibrium

Symbols

C	Total production cost [US$]
C_{alloc}	Allocated cost of utility plants and related facilities [US$]
C_B	Equipment base cost [US$]
$C_{catalyst}$	Cost of catalyst [US$]
C_{cont}	Cost of contingencies [US$]
C_d	Discounted case flow [US$]
C_{DPI}	Direct permanent investment [US$]
$C_{excl\ dep}$	Total production cost excluding depreciation [US$]
C_{land}	Cost of land [US$]
C_P	Purchase cost after inflation adjustment [US$]
$C_{P,base}$	Purchase cost at base year [US$]
C_{royal}	Cost of royalties [US$]
C_{serv}	Cost of service facilities [US$]
C_{site}	Cost of site preparation [US$]
C_{spares}	Cost of spare pumps [US$]
$C_{startup}$	Cost of plant startup [US$]
C_{TBM}	Total bare module investment [US$]
C_{TCI}	Total capital investment [US$]
C_{TDC}	Total depreciable capital [US$]
C_{WC}	Working capital [US$]
COM	Cost of manufacture [US$]
D	Depreciation [US$]
f	Fraction of total depreciable capital
GE	General expenses [US$]
F_{BM}	Bare module factor
NPV	Net present value [US$]
r	Interest rate [%]
S	Total sales revenue [US$]

have also introduced other alternative alkylation processes, but little information is known about them. Hence, liquid-phase zeolite-based alkylation process is selected for the present study.

The EB process consists of reaction section (involving alkylation and trans-alkylation reactions) and separation section to separate benzene, EB, di-EB (DEB), poly-EB (PEB) and trace impurities such as methane and ethane via distillation. Both Woodle (2006) and Welch et al. (2005) have summarized key design features of industrial EB plants. Luyben (2002, 2010) has proposed two similar EB process designs, which use continuous stirred tank reactors (CSTRs) instead of industrial practice of using plug flow reactors (PFRs) and also ignore PEB formation (due to unavailability of reaction kinetics), thus requiring fewer distillation columns for separation. Ebrahimi et al. (2011, 2012) suggested a different design for EB process with three packed-bed adiabatic reactors in the reaction section and four columns in the separation section. In all designs, alkylation and trans-alkylation reactions occur in separate reactors to improve process efficiency (Gerzeliev et al., 2011). Guidelines and ranges for operating variables such as benzene to ethylene (B/E) ratio and temperature are detailed in Woodle (2006) and in Al-Kinany et al. (2012) with reasons elaborated.

Various reaction kinetic models have been proposed for liquid-phase alkylation and/or trans-alkylation reactions by Ganji et al. (2004), Luyben (2002, 2010) and You et al. (2006). Ganji et al. (2004) have also provided plant data of such liquid-phase reactions, which are useful for validation and selection of a kinetic model for reactor design. EB process with conventional distillation columns (CDCs) was studied earlier. Luyben (2010) considered total annual cost as an objective in EB plant design. Ebrahimi et al. (2011) maximized EB selectivity by varying both ethylene feed flow rate and reactor temperature. In the later work of Ebrahimi et al. (2012), objective was the concentration of trans-DEB, which is related to EB selectivity. However, the objectives employed in all these studies do not reflect the performance of the entire process. Although DWC has not been studied for separation of benzene, EB, DEB, PEB and inerts in the EB process, it has been studied for similar systems involving benzene and EB. Premkumar and Rangaiah (2009) reported significant energy and capital savings by using DWC. Gómez-Castro et al. (2008) and Gutiérrez-Antonio and Briones-Ramírez (2009) optimized DWC for multiple objectives. While EB process and DWC have thus been simulated and studied separately, complete EB process with DWC has not been investigated.

The present research has two key objectives. One is to develop and simulate two complete processes for EB production, namely, liquid-phase alkylation using zeolite catalyst, with CDCs or DWC employed for downstream separation. Second objective is to analyse the two EB processes for important objectives: total capital investment (C_{TCI}), net present value (NPV) and benzene loss, which encompass both economic and material indicators of the entire plant. Sensitivity of these objectives with respect to lower/upper bound of decision variables is analysed by using an interface between Microsoft Excel and Aspen HYSYS. New contributions of the present study are development and simulation of an improved, realistic and complete industrial EB process, considering reaction, separation and heat integration aspects. Selected alkylation and trans-alkylation reaction kinetics in the literature are validated with data from an industrial EB plant. Next, two different separation schemes, namely, CDCs and a DWC are studied for recovering the product from the perspective of the complete EB process. Finally, heat integration and sensitivity analysis are conducted for both EB designs. This study shows that EB process using DWC instead of CDCs reduces C_{TCI} by 2.8%, decreases benzene loss by 0.36% and increases NPV by 138%. Hence, DWC is promising for improving sustainability of the EB process.

2. EB process design and simulation

An industrial EB process has 3 main stages: alkylation of benzene to EB in several PFR beds, downstream separation of benzene, EB, DEB, PEB and inerts using two CDCs, and trans-alkylation of DEB to EB in a single PFR bed. The process flow diagrams of the complete processes employing either CDCs or DWC are shown in Figs. 1 and 3, respectively. This study uses plant capacity of 368,000 ton of EB/year, based on typical production rates of new EB plants in Asia Pacific (Woodle, 2006). Operating time is taken to be 8000 h/year and plant life is assumed to be 20 years. Minimum EB purity is 99.95 wt% for the UOP EBOne^{TM} process (Woodle, 2006). However, to satisfy the contract liability in the event of disturbances, a slightly higher EB product purity of 99.97 wt% is set for the design.

Fresh benzene and polymer-grade ethylene are the raw materials for EB process. Fresh benzene is assumed to be