DTU Library

Systematic Approach for Conceptual Process Design: Production of Styrene From Benzene and Ethylene

Cignitti, Stefano; Linnea Franck, Stéphanie; Kepa, Katarzyna; Mattei, Michele

Publication date:
2013

Citation (APA):
Cignitti, S., Linnea Franck, S., Kepa, K., & Mattei, M. (2013). *Systematic Approach for Conceptual Process Design: Production of Styrene From Benzene and Ethylene*. Abstract from 2013 AIChE Annual Meeting, San Francisco, CA, United States.

Systematic Approach for Conceptual Process Design: Production of Styrene from Benzene and Ethylene

Stefano Cignitti[1], Stéphanie Linnea Franck[2], Katarzyna Kępa[1], Michele Mattei[1]
steci@student.dtu.dk, *s072796@student.dtu.dk*, *s120534@student.dtu.dk*, *micu@kt.dtu.dk*
[1]Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229,Søltofts Plads, DK-2800 Kongens Lyngby, Denmark
[2]BioBusiness and Innovation Platform, Copenhagen Business School, Solbjerg Plads 3, DK-2000 Frederiksberg, Denmark

Abstract
Styrene monomer is a highly important and demanded commodity chemical utilized for the production of a large range of polymers and co-polymers including polystyrene, rubber, resin and latex. In this work, a systematic method is utilized to design an economically feasible, sustainable and environmentally acceptable process for the production of styrene from benzene and ethylene. The conceptual process design was performed in the MSc-level course "Process Design: Principles and Methods" at the Department of Chemical and Biochemical Engineering.
In the base case design, styrene is produced by a two-step process, which is extensively used in the industry. The first involves high-pressure alkylation of ethylene and benzene into the intermediate product ethylbenzene. The latter subsequently undergoes dehydrogenation into styrene. The by-product p-diethylbenzene is converted into ethylbenzene by addition of recycled benzene in a transalkylation reactor. Ethylbenzene is recovered along with styrene and the compounds are purified in two sequences of distillation columns.
The systematic method is based on twelve sequential tasks. The first three cover a detailed description of the raw materials, product and process as well as flow sheet synthesis executed by hierarchical decomposition [1]. In task 4, linear mass balance calculations are performed for the synthesized flow sheet. In tasks 5-7, process conditions are specified and mass & energy balance is performed using more rigorous models in order to obtain the base case design. Subsequently, in tasks 8-9, sizing and costing are estimated. In the final three tasks, the process is improved through heat integration, sustainability and environmental impact analysis and process optimization.
A commercial simulator is used for verification and process simulation, together with other computational tools: *ICAS* for property prediction, *ECON* for cost estimation of the process [2], *SustainPro* for sustainability analysis and bottleneck identification [3], *LCSoft* for lifecycle assessment [4].
The following results were obtained from the base case design. The production rate is 500,000 metric tons per year with a yield of 0.6 kg product per kg raw material. The annual revenue amounts to USD 80 million with break-even after 4.5 years. The bottlenecks are the operating cost of a compressor (69%) and the large steam utility of the heat exchangers (17%). These have been overcome by heat integration and process optimization. The total energy consumption amounts to 46.3 kJ per kg product. After heat integration, the external utilities are reduced by 88%.

References

[1] Douglas, J., "A hierarchical decision procedure for process synthesis", *AIChE Journal,* 31, 353-362, 1985.
[2] Peters, M. S., Timmerhaus, K.D., West, R. E., "Plant Design and Economics for Chemical Engineers",*McGraw-Hill,* 2004.
[3] Carvalho, A., Matos, H.A., Gani, R., "SustainPro-A tool for systematic process analysis, generation and evaluation of sustainable design alternatives", *Computers and Chemical Engineering*, 50, 8-27, 2013.
[4] Piyarak, S., "Development of software for Life Cycle Assessment", The Petroleum and Petrochemical College, Chulalongkorn University, Thailand, 2012.