An Investigation into Reactor Type for Bibenzyl Production

A comparison of CSTR and batch reactor for a bibenzyl chemical plant and the designing of the separation process on behalf of Albemarle.

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Background Information

- Diphenylethane (DPE) is produced by a synthesis reaction of benzene with dichloroethane (EDC). DPE has two isomers: 1,1-DPE and 1,2-DPE (a.k.a bibenzyl).
- Bibenzyl is a key chemical used by Albemarle to produce flame retardant coatings after undergoing bromination.
- The Friedel-Crafts synthesis reaction is catalyzed by aluminum chloride. The catalyst is rendered inert by washing the crude product with water producing aluminum hydroxide and hydrochloric acid.
- HCl is corrosive to metal thus Hastelloy B-3 was selected as a construction material due to its resistance to HCl corrosion at all concentrations and up to 100 ℃
- The production of brominated DPE was not considered for this study and the cost assumed to be negligible.
- A comparison of capital cost of the CSTR and the batch reactor shows that the batch reactor model to be more economically feasible; an approximate $1 million difference.

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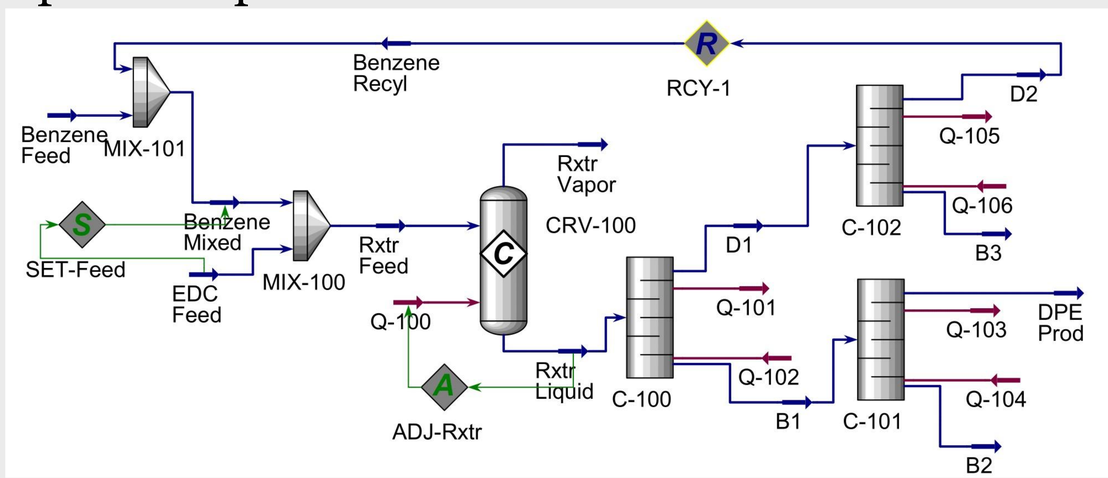

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Continuous Stirred Tank Reactor

- A CSTR is a reactor that maintains steady state flow and mixes the solution while facilitating the reaction.
- The purpose of the mixer is to ensure equal concentrations of reactants throughout the solution which improves the conversion of reactants into desired products and the reaction rate, as well as suppresses formation of undesired byproducts.
- The CSTR modeled will produce 40,237 lbs of DPE per day.
- The total reactor volume is 14,640 L, which was calculated using second order kinetics.
- The CSTR material volume is 0.61 m^3 with 20mm thick walls.
- Using the necessary volume of Hastelloy B-3 to construct the reactor will have a capital cost of $1.2 million.

Batch Reactor

- A batch reactor is a vessel in which reactants are added at the beginning of the reaction and allowed to react for a predetermined amount of time.
- No feed is added or product withdrawn.
- The batch reactor modeled is equipped with an agitator to maintain equal concentration throughout.
- The reaction time is 118 minutes per batch.
- The required volume for the batch reactor is 6475 L based on 2nd order kinetics and reactor design equations.
- For a 20 mm thick reactor wall, the required amount of Hastelloy B-3 is 0.322 m^3.
- The total capital cost for the batch reactor is $624,000 including a factor of 7 to account for installation.

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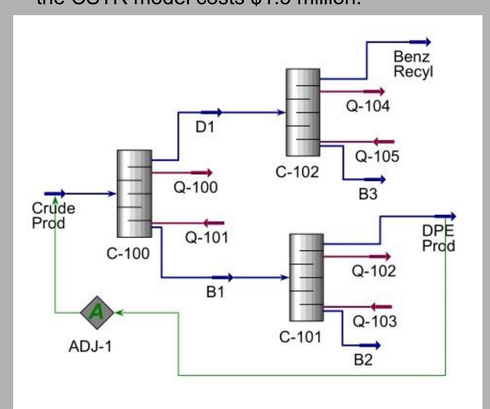
DPE Purification

- The synthesis of DPE produces multiple side products that must be removed to produce a product with 99.95 purity. Notably: toluene, ethylbenzene, 1,1,2-triphenylethane, and 1,1,2,2 tetraphenylethane.
- Distillation columns were selected as the best method of separation due to the sizable differences in boiling points between side products and DPE.
- Aspen HYSYS was used to develop the purification processes for the CSTR and batch models.
- Purification of DPE from side products for both models required two columns.
- A third column was added to both models for the purification and recycling of benzene from light key side products.
- The purification systems for the batch model cost $1.04 million. The purification system for the CSTR model costs $1.5 million.



Acknowledgements
The authors would like to thank Dr. Kevin Caple and Dr. Rahit Lusianti of Albemarle and Dr. Nicholas AuYeung and Dr. Patrick Geoghegan of Oregon State University for their assistance with this project.