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Making the Most of Every Molecule through CRE and Systems Engineering: Molecular Management in the Aromatics Complex

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Highlights

- EB Isom catalyst requires dedicated separation to preserve reaction intermediate
- Utilized molecular management to ensure yield and reactor efficiency
- Confirmed catalyst performance under modified feed and risk conditions
- New design results in reduced capital and utility expenses for aromatics complex

1. Introduction

Para-xylene, the main feedstock for polyester fibers, resins, and films, is one of the most important petrochemical intermediates produced from an overall aromatics complex designed to convert upstream petroleum naphtha. UOP is a leading licensor of aromatics technology and offers process configurations comprising conversion of a mixed aromatics stream to xylenes and separation technology to produce para-xylene.[1] The UOP Parex™ process performs para-xylene separation via a simulated moving-bed separation process.[2] Toluene is one possible desorbent used to selectively displace components from adsorbent chambers to extract and raffinate streams; distillation is required to separate the desorbent from the xylene products and recycle back to the process. Using toluene compared to heavier desorbent chemicals results in lower capital expenditures by streamlining xylene fractionation and removing the need for a separate desorbent supply, as toluene is a by-product of other processes within the same aromatics complex.

After para-xylene is selectively separated from ortho- and meta-xylene as an extract, the raffinate stream is sent to the UOP Isomar™ process to re-establish an equilibrium mixture of xylenes for future separation. The Isomar catalysts isomerize xylenes as their main function and process ethyl-benzene (EB) by either deakylating to form benzene or isomerizing to produce xylenes via a naphthenic intermediate. The EB isomerization-type catalysts are the appropriate choice when the main goal of the complex is to limit benzene production and maximize para-xylene production; however, the naphthenic intermediate must be maintained in the reactor feed to suppress excess formation of naphthenes and maintain para-xylene yield.[3]

The combination of Isomar EB isomerization technology and the toluene desorbent Parex process creates a separation challenge as the naphthenes must be preserved within complex circulation but not be allowed to accumulate with co-boiling toluene desorbent, potentially harming separation efficiency. The presented work details a modified separation process to facilitate the integration of the Isomar EB Isomerization reactor into the overall aromatics complex and presents steps taken to ensure robust catalytic performance.

2. Methods

UniSim® Design simulation software was used to model the distillation, separation, and catalytic processes for the Aromatics Complex. Equipment costs were calculated using Aspen Process Economic Analyzer. Utility and techno-economic calculations were performed with proprietary UOP analysis tools.

3. Results and discussion

Figure 1 contains a flow scheme diagram presenting the new aromatics complex design. Initial attempts to preserve the naphthene circulation to Isomar focused on distillation, removing the necessary molecules via a column sidedraw or adding an extra recycle column to handle lighter components. However, the close boiling point range of toluene and the eight-carbon naphthenes proved difficult to efficiently separate, leading either to reduction in para-xylene yield or excessive toluene in the feed to the Isomar reactor. A solution was found utilizing UOP Sulfolane™ technology to recover aromatics from hydrocarbon mixtures. By adding a dedicated extractive distillation column to process the recycle stream, a purified naphthenic stream was recycled back to the Isomar reactor, effectively bypassing the Parex process.

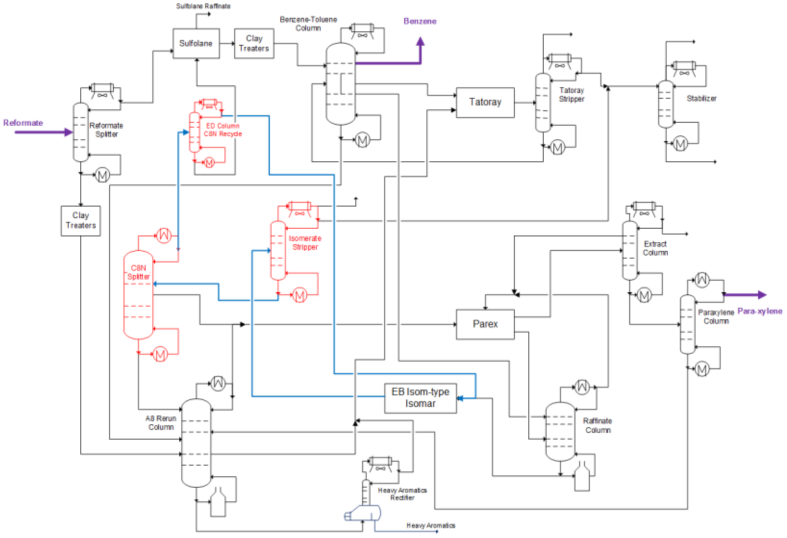

Figure 1. Isomar EB Isomerization reactor integrated into full aromatics complex. Red highlighting denotes new or modified equipment and blue highlighting tracks naphthene circulation through the complex.

As a necessary feature of the new design, the feed to the Isomar unit was modified from the original design conditions of the catalyst. More toluene was expected to reach the Isomar unit via the Parex raffinate stream, as well as higher proportions of heavier aromatic species. Experimental results showed that the elevated components had no adverse impact on the xylene isomerization, EB conversion or ring loss attributes of the catalyst performance. Risk assessment for catalyst life was also investigated related to the Sulfolane process in the event of a process upset; contamination testing results indicated that while there was a significant impact to EB conversion, it was temporary and fully reversible.

Finally, the techno-economic analysis for the design had favorable results: compared to the base case, the modifications represented an 11% reduction in capital expenditures and a 6% reduction in utility costs, leading to an improvement in cash cost of production with similar feed usage and with no negative impact to the catalyst performance.

4. Conclusions

The combination of Isomar EB isomerization technology with the toluene desorbent Parex process produced a unique separations challenge to maintain para-xylene yield while taking advantage of benefits of the lighter desorbent. Through careful molecular management and detailed simulation work, a new aromatics complex was designed that achieved capital expense reductions, lower energy usage, and quality catalytic performance compared with our next-best alternative.

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Keywords
Molecular management; ethyl-benzene isomerization; para-xylene; aromatics complex

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PROFILE

Motivated and detail-oriented scientist and engineer with experience in process development, process modeling and optimization, computational modeling concepts, and microkinetic modeling techniques.

EDUCATION

Northwestern University, Evanston, IL **Graduation Date: 08/2012**
Ph.D. Chemical and Biological Engineering
Kellogg School of Business Management for Scientists and Engineers Certificate Program

University of Wisconsin-Madison, Madison, WI **Graduation Date: 08/2007**
B.S. Chemical Engineering and Mathematics, Graduated with highest honors

RESEARCH AND DEVELOPMENT EXPERIENCE

Senior R&D Engineer/Scientist 2, Honeywell UOP **02/2015 – present**
Aromatics and Derivatives Development, Des Plaines, IL

- Led multiple projects for aromatics complex optimization efforts
- Contributed to kinetic model development with modeling expertise and experimental support

Senior R&D Engineer/Scientist, Honeywell UOP **07/2012 – 01/2015**
Process Modeling and Optimization, Des Plaines, IL

- Utilized optimization methods and interface design to create new software tools for sales support
- Developed new simulation flowsheets with custom modular reactor extensions to support process development efforts

Graduate Research Assistant, Northwestern University **01/2008 – 07/2012**
Advisor: Professor Linda J. Broadbelt, Department of Chemical and Biological Engineering

- Employed quantum mechanical methods to research and develop selective catalytic methods to convert methane directly to chemical feedstocks (Dow Chemical collaboration)
- Applied microkinetic modeling and quantum mechanical calculation techniques to support experimental efforts of collaborators

Undergraduate Research Assistant, University of Wisconsin-Madison **08/2006 – 06/2007**
Advisor: Professor Manos Mavrikakis, Department of Chemical and Biological Engineering

- Studied exhaust gas molecules on metal surfaces to better understand fuel cell reaction kinetics
- Employed quantum mechanical calculations to study dissociation pathways

Undergraduate Research Assistant, University College London **01/2005 – 06/2005**
Advisor: Dr. George Manos, Department of Chemical Engineering

- Studied deactivation of zeolite catalysts while degrading polyethylene waste
- Organized catalytic reactor experiments and analyzed results using gas chromatography techniques

SELECTED PUBLICATIONS AND PRESENTATIONS

Bjorkman, K. R. "Energy Efficient LD Parex Process Development." 2017 TCO Symposium, Itasca, IL, 2017.

Bjorkman, K. R. "LDPX Process Integration with EB-Isomerization." 2015 TCO Symposium, Itasca, IL, 2015.

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Bjorkman, K.R., L.J. Broadbelt. "Oxidation of *cis*-Cyclooctene on Heterogeneous Mn-tmtacn Catalysts." 7th International Conference on Chemical Kinetics, Cambridge, MA, 2011.

Bjorkman, K.R., L.J. Broadbelt. "Oxidation of *cis*-Cyclooctene on Heterogeneous Mn-tmtacn Catalysts: Computational Methods for Reaction Pathway Analysis." 2010 American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, 2010.

INDUSTRIAL EXPERIENCE

Manufacturing Technology/Quality Assurance Intern, 3M Company **05/2006 – 08/2006**
Optical Systems Division, Maplewood, MN

- Executed protective film quality analyses and researched new suppliers, resulting in cost savings

Technical Department Co-op, Georgia-Pacific **06/2005 - 12/2005**
Green Bay Operations, Green Bay, WI

- Collaborated on mill improvement projects to improve process accounting and reduce material costs

LEADERSHIP ACTIVITIES

Technical Community Organization (TCO), Honeywell UOP **2013 - present**

- Participated in program committee to organize and execute annual symposium; led sub-committee to organize networking opportunities
- Elected Chair for 2018 TCO Steering Team; supported committee activities for employee education and community outreach as 2017 Chair-Elect

Graduate Student Association (GSA) President, Northwestern University **2010 - 2011**

Graduate Student Instructor for Summer Technology and Engineering Program (STEP), Northwestern University **2010, 2011**

McCormick Graduate Leadership Council (MGLC) Representative, Northwestern University **2008 - 2010**