Abstract

Process Economics Program Report 1F

ALIPHATIC DIISOCYANATES PROCESSES

(February 2002)

Aliphatic and cycloaliphatic diisocyanates (functional groups –N=C=O) are major building blocks in the manufacture of polyurethane products, which are formed by the controlled polyaddition of the diisocyanates with either polyether or polyester polyol coreactants. These diisocyanates are consumed primarily in non-yellowing, high-performance industrial and automotive polyurethane coatings applications.

Industrial scale production of aliphatic and cycloaliphatic diisocyanates has previously been accomplished by the phosgenation of the diamines. However, in recent years, there has been no lack of attempts to prepare these diisocyanates by phosgene-free processes commercially mainly because of phosgene's corrosivity, high toxicity and high chlorine content. In the mid-1990s, Degussa (previously Creanova or Huls) started-up a 20 million lb/yr IPDI unit in Theodore, Alabama, employing its proprietary phosgene-free urea-based technology; BASF was also believed to have brought on stream a 20 million lb/yr HDI/IPDI swing plant in Germany using a similar patented phosgene-free process.

This report, our sixth on the topic of isocyanates since 1967, presents a comprehensive assessment of the status of the aliphatic and cycloaliphatic diisocyanates industry, primarily HDI and IPDI. It provides a review of current patents and recent business/technology developments, and evaluates major commercial processes. This report also presents two conceptual process designs and economic evaluations for the production of hexamethylene diisocyanate (HDI) and isophorone diisocyanate (IPDI) using non-phosgene urea-based technologies developed by BASF and Degussa. Also presented are updates of the techno-economics in the production of similar scale HDI and IPDI via conventional phosgenation processes. Results of our economic comparison indicate that the phosgene-free urea-based processes are generally more expensive in total fixed capital than their conventional phosgene-based counterparts. Although raw material costs for the non-phosgenation processes are lower, the higher cost of utilities and capital related fixed costs nonetheless result in product values that are 3–7% higher than those obtained via conventional phosgene processes.

In addition, other aliphatic and cycloaliphatic diisocyanates, such as H_{12}MDI (hydrogenated MDI), are also introduced and discussed briefly in the industry status of this report. Overall, this report encompasses the latest technology and process economics, and it provides a basis for insight into technology trends, and possible enhancement in safety and environmental standards with the new phosgene-free routes in the preparation of HDI and IPDI.

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