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TDI (Toluene Diisocyanate) Process Update

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Abstract

Isocyanates are a major ingredient for production of polyurethane products that are formed by the reactive polymerization of isocyanates with polyols. A long and difficult search for a reasonable economic pathway to commercially produce isocyanates by vapor-phase phosgenation of toluene diamine (TDA) in place of liquid-phase phosgenation has been developed and commercialized since our last integrated report on isocyanates (PEP Report 1E) was published in August 1992.

Isocyanates are produced in large quantities and serve mainly as starting materials for the production of polyurethanes. They are usually prepared by reacting the corresponding amines with phosgene. One way of producing isocyanates is the reaction of the amines with phosgene in the gas phase. This is usually referred to as a gas-phase phosgenation process, characterized by the fact that the reaction conditions are selected so that at least the reaction components amine, isocyanate, and phosgene—but preferably all reactants, auxiliary agents, products, and reaction intermediates—are gaseous under the conditions selected. Advantages of gas-phase phosgenation include reduced phosgene holdup, avoiding difficult phosgenate intermediates, and increased reaction yields.

In this review, we investigate large-scale, single-train integrated technology and economics for production of toluene diisocyanate (TDI), including nitration of toluene to produce dinitrotoluene (DNT), hydrogenation of DNT to produce toluene diamine (TDA), production of phosgene from carbon monoxide and chlorine, gas-phase phosgenation of TDA to produce crude TDI, separation/recovery of TDI products, and possible hydrolysis of TDI tars to recover and recycle TDA. The key gas-phase phosgenation step produces isocyanates from TDA at high pressure and temperature, enabling a significant shortening of residence time in the reactor. The rate-determining phosgenation step is the dissociation of the polymeric TDA–carbonyl chloride intermediate into polymeric TDI and HCl, followed by HCl removal.

A summary of the process economics for production of 300,000 metric tons/year (660 million lbs/year) of TDI by continuous vapor-phase phosgenation shows that on a US Gulf Coast basis, a world-scale, single-train, integrated vapor-phase technology–based plant will easily meet plant gate costs. On the same basis, a world-scale, single-train plant will also approximately meet net production costs. With lower capital and manufacturing costs—for example, in China—manufacturing operations would likely be more profitable. The Bayer MaterialScience plant in China is the first to use new gas-phase phosgenation technology at world scale. The goal for this technology is reported to be able to run at a turndown capacity of about 50% of full rate without reducing product quality, which means that a plant can be far more responsive to market demand without the need for multiple plants.

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