

CHEMSYSTEMS PERP PROGRAM

Adipic Acid

Technology and Cost Estimates for Adipic various Acid Production Technologies: Commercial Routes involving KA and subsequent nitric acid oxidation; a process involving integrated nitrous oxide oxidation of benzene; speculative butadiene routes via carbonylation, and direct oxidation of cyclohexane with air/oxygen; а conceptual design based on а biosynthetic route. Regional supply, demand and trade forecasts are included.

PERP 08/09-2

Report Abstract February 2010

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INTRODUCTION

Current commercial processes to produce adipic acid are carried out in two stages: (1) Production of cyclohexanone or cylohexanol, or a mixture of both, (i.e., KA - K for ketone and A for alcohol); and (2) subsequent conversion to adipic acid.

The chemistry mainly involves the production of the KA mixture in the first step, since there are various routes to yield this intermediate; unlike the second step conversion to adipic acid, which nowadays is almost always by reaction with nitric acid (prior to Dupont's introduction of this procedure some seventy years ago, it had been carried out by air oxidation). The nitric acid oxidation of KA oil produces significant quantities of nitrous oxide (N₂O), and NOx (NO, NO₂, and higher oxides). NOx effluent has been regulated for many years. Treatments to recover or remove NOx are employed in all existing plants. Nitrous oxide abatement is discussed in this report.

The chemistry of the commercially employed routes is pictured in the upper portion of the figure shown below. Alternative and developing routes are summarized in the lower half of the figure.

Proof of concept has apparently been achieved for production of adipic acid from an alkane feedstock by a fermentation process using a yeast microorganism. Parallel research to engineer improvements to a proprietary metabolic pathway that allows the microorganism to utilize sugar and plant-based oils feedstocks as well as alkanes is ongoing.



Routes to Adipic Acid



COMMERCIAL TECHNOLOGY

It is generally considered that the main commercial route employed for production of KA is the oxidation of cyclohexane, employed by producers such as DuPont, BASF and Stamicarbon. There are three main variations to this basic cyclohexane oxidation process. The oldest process still in use is cobalt-catalyzed oxidation. The other two variations are known as the high peroxide process and the boric acid promoted oxidation process.

Another large-scale commercial technology used to produce KA oil is by phenol hydrogenation. Adipic acid producers that use phenol-based production technology include DSM, Radici and Inolex. Phenol is either purchased, or produced on site by cumene or toluene.

Around 1990, Asahi commercialized the production of cyclohexanol from cyclohexene, an intermediate obtained from the partial hydrogenation of benzene. Oxidation of the produced cyclohexanol results in adipic acid.

The chemistry and technology (including process flow schemes) of all these processes are discussed in the report.

ALTERNATIVE AND EMERGING TECHNOLOGIES

A number of alternative and developing processes are discussed in the report, in particular:

- Adipic Acid Production Incorporating Integrated Nitrous Oxide Oxidation of Benzene
- Direct Oxidation of Cyclohexane Using Air/Oxygen
- Adipic Acid Production via Butadiene Carbonylation
- Biosynthetic Production of Adipic Acid using an *E.coli* host (conceptual design)

ECONOMIC ANALYSIS

The following cost of production estimates have been developed:

- Adipic Acid Production Via Boric Acid Promoted Oxidation of Cyclohexane To KA Oil.
- Adipic Acid Production Via Cobalt Catalyszed Oxidation of Cyclohexane To KA Oil.
- Adipic Acid Production Via Hydrogenation of Phenol To KA Oil.
- Adipic Acid Production Via Benzene Partial Hydrogenation/Cyclohexene Hydration To Cyclohexanol.
- Adipic Acid Production Via Hydrogenation Of Phenol To KA Oil Incorporating Integrated Nitrous Oxide Oxidation of Benzene (Solutia Process).
- Adipic Acid Production by Direct Oxidation of Cyclohexane Using Air Only (BASF Process).
- Adipic Acid Production By Butadiene Carbonylation.

The sensitivity of the cost of production to the primary feedstock price has been carried out.

• Based on a conceptual design, a speculative first approximation estimate of the cost of producing adipic acid via a biosynthetic route using an *E.coli* host has been estimated

MARKET ANALYSIS

The main uses of adipic acid are for nylon 6,6 fiber and resins, with much lesser amounts going into polyester polyols used in polyurethanes and into adipic acid esters, which serve as specialty plasticizers as exemplified in the figure below. Nylon 6,6 fiber is used in carpet yarn, home furnishings, apparel, tire cord, fishing lines, brush bristles, parachutes, and backpacks.



North American Adipic Acid Demand by End-Use

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- This report gives a discussion on regional supply, demand and trade data for North America. Western Europe, Japan and China.
- Tables giving individual plant production capacity according to plant location, plant owner, and feedstock for the regions listed above are also included.





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