Isoprene/Bioisoprene

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Nuno Faísca and
Caleb Chong Wei Ping

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Mrs. Heidi Junker Coleman, Global Support Manager, Multi-Client Programs: phone +1 914 609 0381 and e-mail hcoleman@nexant.com

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INTRODUCTION

Isoprene (2-methyl-1,3-butadiene) is an important commodity chemical with annual demand of over a million tons per year. Most isoprene is consumed in the production of polyisoprene (via polymerization of isoprene). Polyisoprene (Isoprene Rubber, IR), is similar in structure and properties to natural rubber. Polyisoprene is largely used in the manufacture of vehicle tires (or tyres). (It is interesting to note that after so many developments in the tire industry, natural rubber (or polyisoprene) remains a crucial ingredient in the manufacture of quality tires, mainly because of its ability to resist the heat build-up generated by friction.) Styrene-isoprene-styrene copolymer (SIS Rubber), is the second largest application of isoprene and it is mainly used as a thermoplastic rubber and as a pressure-sensitive or thermosetting adhesive. In smaller amounts isoprene is also used in the production of butyl rubber, isobutylene-isoprene copolymer (IIR). Isoprene has some use as an intermediate for the production of specialties. The companies that consume isoprene for the production of specialties include Kuraray, Nissan Chemical, Takasago, and Rhodia (now Solvay).

Structurally, isoprene may be represented as below:

![Isoprene Structure](image)

A major focus of this PERP report is to detail the process technologies and costs of production of manufacturing isoprene using the emerging fermentation processes as compared to the conventional process of extracting isoprene from Cs streams, and on-purpose routes to isoprene.

The report also gives commercial market analysis – commercial applications and supply/demand market analysis globally and broken down according to key regions; as well as an overview of strategic considerations of being in the isoprene production business.

TECHNOLOGY

Over the years, many process technologies have been investigated for isoprene production. A summary of the process technologies reviewed in this report for the production of isoprene is given in the table below.
Routes via C₅ Streams

The production of isoprene from C₅ streams is currently the preferred route to isoprene. The C₅ feed stream, independent of its source, is a mixture of components with different commercial importance.

The C₅ compounds of commercial interest can be divided into diolefins or dienes and olefins. This division is important because, as is described in the report, it corresponds to two distinctive feedstocks in the production of isoprene. Whilst, isoamylenes (e.g., 2-methyl-2-butene, 2-methyl-1-butene) and 1-pentene are the olefins in the C₅ feed stream with higher demand, the C₅ dienes used commercially are isoprene, cyclopentadiene (generally used as its dimer dicyclopentadiene – [i.e., DCPD]), cis and trans-1,3-pentadiene (cis and trans-piperylene).

There are three main sources of C₅ feed streams:

- Unsaturated (“raw”) pyrolysis gasoline – by-product of hydrocarbon steam cracking
- Product stream from the Fluid Catalytic Cracking Unit (FCCU) in refineries
- Natural Gas Liquids (NGLs), (i.e., condensates)

Isoprene cannot be isolated from the C₅ cracking fraction by simply utilizing a set of distillation columns because, (i) the C₅ stream comprises many other components which have very similar boiling points to isoprene, and (ii) isoprene and n-pentane form an azeotropic mixture. Extractive distillation processes are all based on the same principle, the addition of a solvent that forms no azeotrope with the remaining components in the mixture. The added solvent interacts differently with the different components of the mixture, changing their relative volatilities, and consequently, facilitating the distillation of the mixture.

There are two main process technologies available to produce isoprene from C₅ streams:
These two main processes are discussed in detail in the report, and in addition, the first-stage hydrotreatment process technology typically employed before sending the C₅ stream to the gasoline pool, is also reviewed. Although, this first-stage hydrogenation process is not relevant in the production of isoprene, it is important to understand the process because of the methodology employed in the development of the process economics (i.e., to determine gasoline blending values).

Commercial technologies discussed in the report include:

- Hydrotreatment of the Mixed C₅ Stream
- Extractive Distillation Process Technology
- Isopentane Dehydrogenation Process Technology

Since isoprene is typically produced using a complex series of extractive distillation columns, to separate cyclopentadiene and its dimer dicyclopentadiene (DCPD), and subsequently piperylene. This is a relatively expensive and energy-intensive process (despite having valuable byproducts). Furthermore, with the recent developments in shale gas and fracking technology, most steam crackers in North America, for example, are shifting to lighter feedstocks (i.e., ethane), decreasing the availability of C₅ cracking streams.

**On-Purpose Routes**

With the worldwide demand for isoprene expected to increase and with a lower availability of C₅ streams, the cost of isoprene is expected to rise to much higher levels. The current isoprene market growth is constrained by supply. Moreover, the C₅ cut stream has a high octane value making this raw material difficult to secure and costly for petrochemicals. Consequently, there is a consensus that the petroleum-derived isoprene will be insufficient to meet world demand and that the isoprene price will escalate to unprecedented values. On-purpose routes, such as the new one-stage processes licensed by EuroChim and Kuraray are expected to be of critical importance to balance the isoprene market demand. Acetylene-based technology (i.e. Snamprogetti Process) is also included in the report because it may have a role to play in the Chinese industry, emulating what happened in the production of vinyl acetate and vinyl chloride monomers.

In summary the on-purpose commercial routes discussed in the report include:

- Two-stage isobutylene carbonylation process technology (conventional m-dioxane route)
- One-stage isobutylene carbonylation process technology (Eurochim and Kuraray)
- Acetone-Acetylene Process Technology (Snamprogetti Process)
- Goodyear/Scientific Design Proprietary Propylene-Based Route

Patents published by Phillips and Lyondell describing olefin metathesis/dismutation technology are reviewed.
Bioroutes

Industrial biotechnology (or “white” biotechnology) has never been so eminent to play a key role in chemical processes. The present conjecture of drivers, breakthroughs in synthetic biology and the steadily increase in oil prices, results in a crucial moment for investments in industrial biotechnologies.

It is increasingly evident that the petrochemical-derived isoprene (“petro-isoprene”) faces challenging times with the foreseeable rise in oil price. The recent announcements of partnerships between major downstream rubber players and biochemical companies (e.g., Ajinomoto-Bridgestone, Amyris-Michelin, and DuPont-Goodyear) are not surprising. Other companies developing fermentative isoprene processes are GlycosBio, Aemetis, and LanzaTech. It is an excellent opportunity for non-petroleum based technologies, and even more for industrial biotechnology investments (biomass-based feedstock).

In 2009 Genencor (now DuPont) delivered the first biologically derived isoprene to their partners, Goodyear, for the production of tires.

In this section of the report:

- The biochemistry underlying the production of isoprene is given, and highlights the fermentative pathways, yields, renewable feedstocks, and selected isoprene producing organisms
- A conceptual process design for producing isoprene is given detailing steps from inoculum preparation to the plant reaction and separation/purification sections
- Licensor and other key players are discussed

PROCESS ECONOMICS

The report includes detailed cost of production estimates for world scale, state-of-the-art, isoprene plants. The selected cases are:

- Cost of producing isoprene via on-purpose technologies
  - Snamprogetti Process (China location basis)
  - Isobutylene Carbonylation (2-Stages) Process (China, N.W. Europe, USGC location bases)
  - Isobutylene Carbonylation (1-Stage) Process (China, N.W. Europe, USGC location bases)

- Cost of producing isoprene via C₅ streams
  - Extractive Distillation (China, N.W. Europe, USGC location bases)
  - Isopentane Dehydrogenation (China, N.W. Europe, USGC location bases)

- Cost of producing isoprene via Bioroutes
  - Fermentation via MVA Pathway (N.W. Europe, S.E. Asia and U.S. Midwest location bases)
  - Fermentation via DXP Pathway (N.W. Europe, S.E. Asia and U.S. Midwest location bases)
Fermentation via Optimized MVA Pathway (N.W. Europe, S.E. Asia and U.S. Midwest location bases)

The detailed cost tables given in this report include a breakdown of the cost of production in terms of raw materials, utilities consumed (electrical energy, cooling water, fuel etc.), direct and allocated fixed costs, by unit consumption and per metric ton and annually, as well as contribution of depreciation to arrive at a cost estimate. Capital costs are broken down according to inside battery limits (ISBL), outside battery limits (OSBL), other project costs, and working capital.

COMMERCIAL MARKET REVIEW

A description of the main isoprene derivatives and their respective commercial applications is given in the report, i.e., Polyisoprene Rubber (IR), Styrene-isoprene-styrene (SIS), Butyl Rubber (IIR), Specialty chemicals, including synthetic production of terpenoids from isoprene, and the potential of isoprenoid-based fuels is discussed. The Figure below illustrates global demand of isoprene according to its end-use application.

![Global Isoprene Demand by End-Use](image)

The report includes market analysis as follows:

- Global supply, demand and trade data is given and discussed
- In addition, supply, demand and trade data is given and discussed according to key regions, i.e., North America, Western Europe, Central and Eastern Europe, Asia Pacific, and Rest of the World (i.e., South America, and Middle East and Africa).
- Tables giving all production plants known to Nexant showing specific plant capacities, owning company, and location of plant
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