

Bio-Routes to *para*-Xylene

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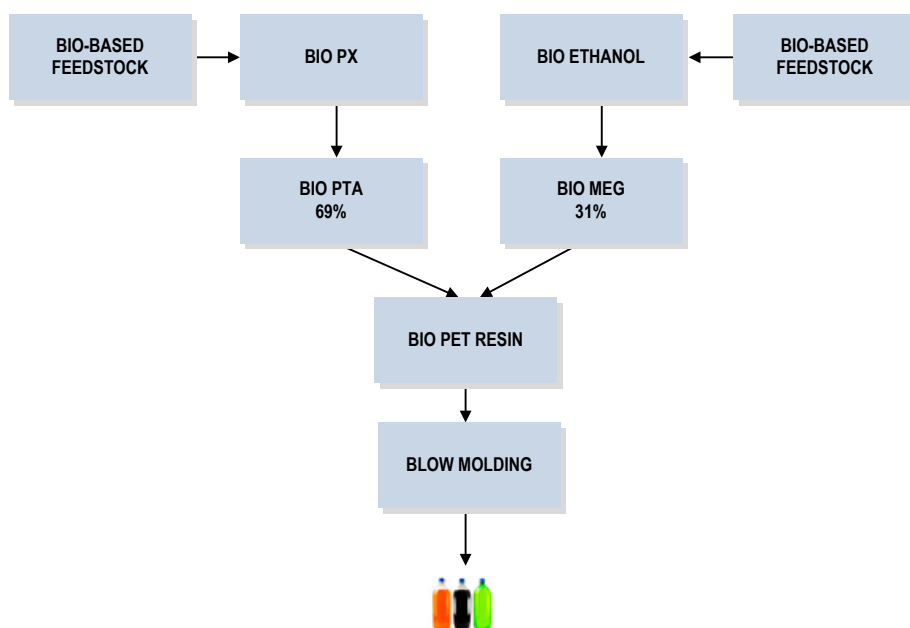
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INTRODUCTION

The possibility of a renewable source of *para*-xylene (the feedstock for terephthalic acid (PTA)), which is in turn a monomer, along with monoethylene glycol (MEG), for bottle resin polyethylene terephthalate (PET)) is important to the entire global sectors concerned with food packaging and textiles (for PET fiber). High resin prices have increased the need to create totally “green” PET bottles as replacements for petroleum-derived ones. This has led to recent announcements by H.J. Heinz Company for plans to use Coca-Cola’s 30 percent plant-based PET PlantBottle™ for packaging its ketchup; PepsiCo which announced a 100 percent plant-based PET bottle in the laboratory; and renewable chemical technology firms Gevo, Virent and Avantium to help Coca-Cola develop a 100 percent plant-based polyethylene terephthalate (PET) resin for its PlantBottle™ packaging. Although PET is recycled already (but at an average of only 28.0 percent in 2009), by producing a “green” PET from renewable *para*-xylene and MEG, one can claim a better environmental impact and simultaneously reduce our dependence on oil. The technology for making “green” or bio-based ethylene glycol from bioethanol has long been commercialized and is discussed in PERP report 09/10S8 *Green Glycols and Polyols*.

How to Make 100 Percent Renewable PET*



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* adapted from Coca Cola web site graphic http://www.thecoca-colacompany.com/citizenship/plantbottle_basics.html

Within the last year, three bio-options have appeared on the horizon, Virent Energy Systems, Inc.; Gevo, Inc.; and Anellotech, Inc. These three options are very different from one another. The processes operated by Virent and Gevo, are liquid phase, work at relatively low temperatures, and feed on sugar solutions or hydrolysate (at least in the near term), while the

Anellotech's process is a higher-temperature pyrolysis that feeds on wood chips, saw dust, or other ground up biomass. Virent and Anellotech's processes rely on mineral catalysis for their primary and unique conversion step, while the Gevo process is fermentation-based. Anellotech and Virent produce their hydrocarbon products in essentially one step, while Gevo requires three subsequent stages of catalytic conversion to go from its primary product, bio-isobutylene, to *para*-xylene. Virent has been salient for several years, Gevo for slightly less time, and Anellotech has only appeared in 2009.

The degree of corporate and technical development roughly parallels this chronology:

- Anellotech is still at the demonstration plant stage
- Gevo has its isobutanol process operating but still needs to demonstrate the ring closure process step commercially
- Virent has a pilot plant operating in Texas and has an advantage in being able to convert both C₅ and C₆ sugars to aromatics

BIOTECHNOLOGY

Anellotech's Biomass to Aromatics™ is based on science research by Prof. George Huber's research lab at the University of Massachusetts-Amherst. The biomass (i.e., wood waste, corn stover, sugar cane bagasse, etc.) is first dried and ground before being injected into a fluid-bed reactor in the presence of a zeolite catalyst. In this one brief step, biomass is rapidly heated without oxygen and the resulting gases are immediately catalytically converted into aromatic hydrocarbons. Other than the reactor, regenerator and the catalyst, the process equipment is conventional equipment found in many chemical facilities.

Gevo is focused on the development of advanced biofuels and renewable chemicals based on isobutanol and its derivatives. Gevo's technology enables the cost effective, practical production of renewable hydrocarbons such as isooctene and isooctane for the gasoline market, renewable jet fuel and renewable diesel blendstocks. In addition, Gevo's technology enables the production of a wide variety of chemicals such as isobutylene and *para*-xylene from renewable resources.

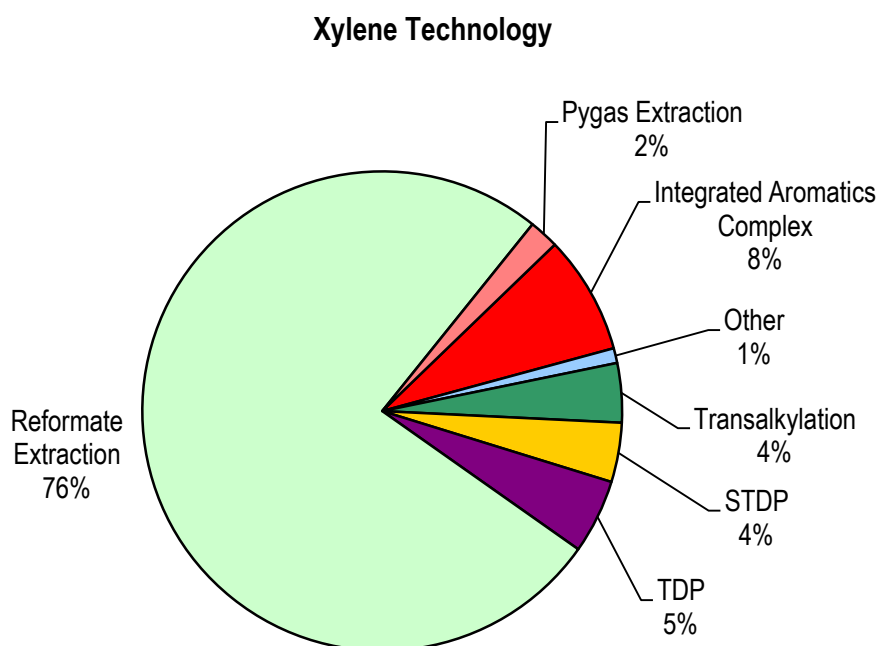
Virent claims that their BioForming® process can convert a wide range of biomass-derived feedstocks to fuels and chemicals. The BioForming® process is based on the Aqueous Phase Reforming (APR) pathway combining catalyst and reactor systems similar to those found in refineries. BioForming® is optimized for the conversion of an individual feedstock to a defined end product among many possible combinations. Sponsors of Virent's development include Shell, Honda Motor, Cargill, Venture Investors, Stark Investments, and Advantage Capital. Its collaborator is the University of Wisconsin-Madison.

Although the report focuses on the research of Anellotech, Gevo, and Virent, other companies doing research in this area include Global Bioenergies, UOP, Pacific Northwest National Laboratory (PNNL) and Washington State University (WSU). Their work is discussed briefly in the report.

COMMERCIAL TECHNOLOGY

The xylene isomers, *meta*-xylene, *ortho*-xylene and in particular *para*-xylene, are important chemical intermediates. *ortho*-Xylene is oxidized to make phthalic anhydride which is used to make phthalate plasticizers among other things. *meta*-Xylene is oxidized to make isophthalic acid, which is used in unsaturated polyester resins (UPR). However, *para*-xylene has by far the largest market of the three isomers. The largest use of *para*-xylene is in its oxidation to make terephthalic acid. Terephthalic acid is used in turn to make polymers such as polyethylene terephthalate (PET) and polybutylene terephthalate (PBT). PET is one of the largest volume polymers in the world. As such, the demand for *para*-xylene is several times that for *meta*- and *ortho*-xylene.

Xylenes are normally obtained from various sources within a refinery or steam cracker including reformat, pyrolysis gasoline, toluene disproportionation, and transalkylation. Globally, reformat accounts for over 75 percent of the mixed xylenes. These sources usually produce a mixture of isomers from which the individual isomer is recovered.



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Commercial technology routes to produce *para*-xylene are briefly summarized in this section of the report.

PROCESS ECONOMICS

Cost estimates for *para*-xylene production via the following processes have been evaluated:

- Commercial integrated naphtha to *para*-xylene route for plant capacity of 1 000 kta on a USGC basis.
- Anellotech's speculative (non-commercial) *para*-xylene route for plant capacity of 250 kta plant on a USGC basis.
- Gevo's speculative (non-commercial) *para*-xylene route for plant capacity of 250 kta plant on a USGC basis.
- Virent's speculative (non-commercial) *para*-xylene route for plant capacity of 250 kta plant on a USGC basis

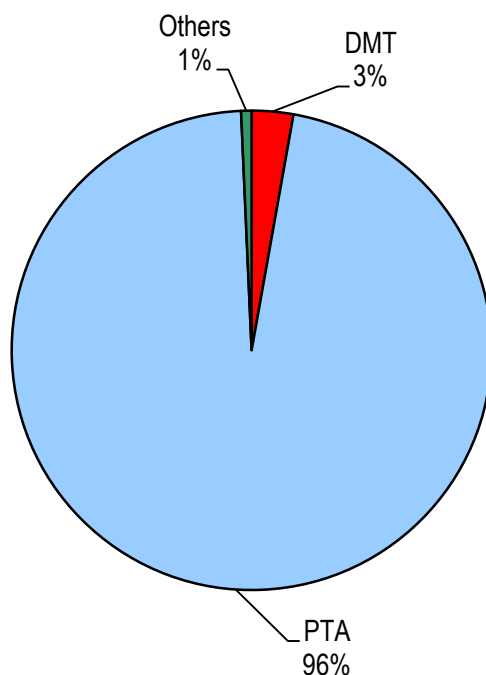
The above cost estimates highlight the different process performances of the speculative routes as they are all compared on a same capacity and location basis. However, other regions reflect to a greater extent the developing industry based on planned new projects. Therefore, Nexant has also developed and compared the economics of production for the Anellotech route to *para*-xylene for Brazil and Western Europe.

In addition, the sensitivity of the economics for producing bio *para*-xylene has been developed for feed price, capital investment, and economy of scale.

All cost tables given in this report include a breakdown of the cost of production in terms of raw materials, utilities 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 (a simple nominal return on capital is also included).

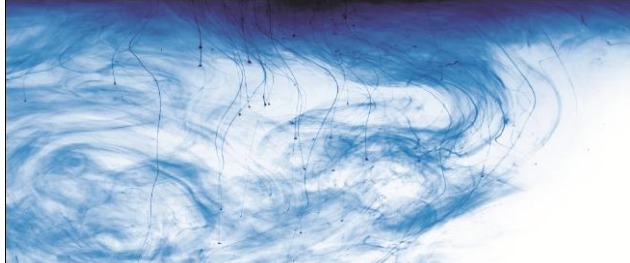
COMMERCIAL ANALYSIS

The global *para*-xylene market can be categorized to three main regional profiles. The mature markets in North America and Western Europe have a low growth outlook for *para*-xylene. Smaller consuming regions such as South America, Eastern Europe and the Middle East have a higher growth outlook, but this is limited in scale due to their reliance on the PET container resin market. Lastly Asia Pacific, which is by far the largest consuming region, and will drive global growth. This is due primarily to the labor cost advantage of producers in the region, which has allowed them to dominate the global PET fiber market, which accounts for around two-thirds of the total global PET demand. China alone now accounts for around two-thirds of the global PET fiber production. The huge populations in Asia are also driving high long term growth rates for PET container resins. Asia Pacific is therefore the real driver of *para*-xylene demand, accounting for roughly 80 percent of the global total.

Global *para*-Xylene End-Use Pattern, 2010

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- Global supply, demand and trade data are given and discussed.
- In addition, supply, demand and trade data is given and discussed according to key regions (i.e., United States, Western European, and Asia Pacific)
- A list of plants in each of the key regions above is given showing specific plant capacities, owning company, location and annual tonnage produced



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