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# BPA-Free Baby Bottle Resins

Process Economics & Production Technology of Eastman's New Generation Tritan™ and other Bisphenol A Free Polymers - Polypropylene, Polyethylene, PEN, PES - used for Baby Bottle Manufacture are Compared with Polycarbonate. Global supply overview and health concerns are also given.

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Report Abstract

December 2009

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## INTRODUCTION

Bisphenol A (BPA) has a structure that makes it suitable as a monomer to produce polycarbonate, epoxy, phenolic, polyester, and other resins. Bisphenol A polycarbonate, produced by the interfacial polymerization of BPA with phosgene, was the first major amorphous engineering plastic commercialized.

Polycarbonate (PC) is an amorphous, clear polymer with high transparency, superior dimensional stability, good electrical properties, good thermal stability, and outstanding impact strength and ductility. It is for these properties that PC has found use in food and beverage containers including the infant care market.

While PC has historically been the resin of choice for the manufacture of infant products, such as baby bottles and sippy cups, the alleged health concerns associated with Bisphenol A has prompted manufacturers of baby bottles to look for other alternatives to the commonly used polycarbonate.

The purpose of this report is to assess several alternative resins currently utilized for the production of baby bottles that do not contain BPA monomer. Hence, the report will focus on several alternatives to polycarbonate such as: High Density Polyethylene, Metallocene Polypropylene, Polyethylene Naphthalate, Eastman's Tritan™ Copolyester, and Polyethersulfone. Process chemistry, technology and economics for each of the polymers are discussed, as well as a review of the properties and supply overview for each of the polymers considered.

## HEALTH CONCERNS OF BISPHENOL A

Bisphenol A (BPA) was first synthesized in 1891, although commercial production in the United States and Europe, didn't start up until 1957 and 1958, respectively. Bisphenol A is primarily used as a feedstock for polycarbonate and epoxy resins. Both of these resins have food-containing applications. Polycarbonate's applications include food containers and water and baby bottles. Epoxy resins are utilized for lining food and drink cans, and for dental sealants.

The use of BPA in food contact materials has made it a target of many human and environmental studies even before its commercial production. Since the 1930s, there have been concerns regarding BPA about its potential to act as an estrogen mimic, and the potentially adverse health effects it may have.

Dental sealants and food can linings are the main sources of potential human exposure. Polycarbonate bottles and dishes are more minor sources; however, polycarbonate-based baby bottles have become a real concern.

Testing in 1997 found no detectable BPA in leachates from soda and beer cans. However, BPA was found to migrate into food from those cans that generally require high temperature (over 212 °F) sterilization, such as cans for vegetables, meat, infant formula, and tomato products. Extracts from such cans had BPA levels averaging 37 ppb.

In June 2000, the Worldwide Fund for Nature (WWF) in the United Kingdom issued a report claiming links between BPA in can linings and baby bottles and reproductive effects. An unpublished study by the United Kingdom government indicates that BPA is released from baby bottles that have been subjected to bottle brushing, dishwashing, or sterilization.

In 2001, European Union scientists classified BPA as a category 2 fertility toxicant. However, the chemical industry declared that BPA was safe to use.

By 2005, studies involving BPA and its possible health risks in humans kept increasing. As a result, studies were brought into question by many scientists. A report published in the Environmental Health Perspectives' Journal analyzed 115 studies performed on the safety of BPA. According to the report, significant effects were found in 94 studies funded by governments. On the other hand, no problems were found in 11 studies paid by industry. With this new report, scientists felt the need for a new risk assessment study involving BPA's safety levels.

The current status of legislation in North America, Europe and Asia are outlined in the report.

## PROCESS TECHNOLOGIES

### Polyethylene

Ethylene as a gas or in solution in a diluent can be polymerized in the presence of a catalyst to form a polymer. The reaction is exothermic according to the following. The heat of polymerization is about 1,400 Btu per pound (800 calories per gram).

$$nC_2H_4 \xrightarrow{\text{Catalyst}} (C_2H_4)n$$

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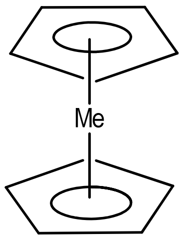
Each of the three generic types (i.e., LDPE, HDPE, and LLDPE) of polyethylene processes is suited to produce a polyethylene with particular characteristics such as density, molecular weight, and molecular weight distribution, as well as degree of polymer crystallinity and branching. However, this report will only look into detail at HDPE, as one of the first applications for HDPE was in the manufacture of baby bottles.

The HDPE technology market is very competitive with numerous technologies competing for each new plant. A brief overview of the technologies available, followed by detailed reviews of three HDPE technologies (Chevron Phillips Slurry Loop, Mitsui Chemical CX Ziegler Slurry and Univation Technologies UNIPOL™ PE Gas Phase Processes) are given in the report. These three technologies account for approximately 58 percent of installed capacity in 2008.

### Metallocene Polypropylene

Metallocenes are organometallic coordination compounds in which transition metals (e.g., iron manganese, titanium, and chromium) are sandwiched between two cyclopentadienyl ligands (in the figure below Me represents a transition metal):

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Metallocene catalysts have the potential to control both molecular weight (distribution) and microstructure (i.e., tacticity, material compositions distribution, stereoregularity, etc.) making the production of new materials, including comonomer systems, possible. Generally, metallocene resins offer the ability to produce a highly stereospecific polymer based on the molecular structure of the catalyst.

Metallocene polyethylene (mPE) technologies to produce some high value elastomer and polastomer grades have been commercially available since 1991, where the commercialization of these technologies into the larger volume polyethylene markets began in October 1995. Commercialization of metallocene polypropylene (mPP), on the other hand, is lagging behind polyethylene.

Metallocene polypropylene polymers are produced in conventional processes using "drop-in" metallocene catalysts.

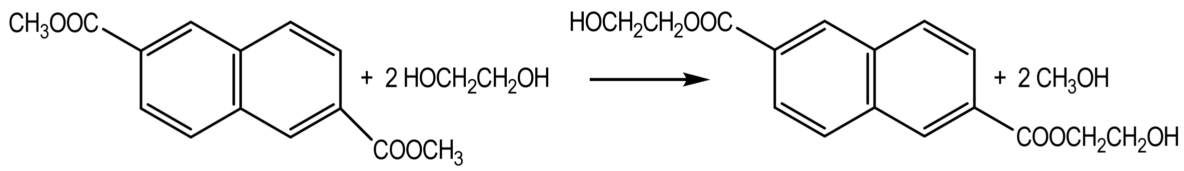
This section of the report refers to the production of metallocene polypropylene via gas phase or bulk loop processes. The Novolen® process (offered by Lummus Novolen® Technology) and the Spheripol (offered by LyondellBasell) have been chosen to represent the technologies available for the production of polypropylene using metallocene catalysts. Clarified polypropylene (cPP) is also discussed in the report since clarified propylene resins are currently being used in the infant care market for the manufacture of baby bottles. cPP is obtained by the addition of clarifying agents to polypropylene resin.

### Polyethylene Naphthalate

Polyethylene naphthalate (PEN) is a high performance polyester whose main advantages over PET are higher temperature resistance, better gas barrier properties, and UV light resistance. The monomers used in PEN production are ethylene glycol (MEG) and dimethyl 2,6-naphthalene dicarboxylate (dimethyl 2,6-NDC).

Dimethyl 2,6-NDC is prepared by oxidation and esterification of dialkyl or alkyl/acyl derivatives of benzene. Early feeds to oxidation were 2,6-diisopropyl naphthalene (made by alkylation of naphthalene with propylene) and 2-methyl, 6-isobutyryl naphthalene. In 1991, Amoco (now BP) developed a process that uses *ortho*-xylene and butadiene as feedstocks for 2,6-dimethyl naphthalene. This and other routes to PEN monomers and their feedstocks are outlined in the report.

The first step in the polymerization sequence is transesterification of dimethyl 2,6-naphthalene dicarboxylate with two moles of ethylene glycol to form 2,6-hydroxyethyl naphthalene dicarboxylate (naphthalate oligomer) and two moles of methanol:

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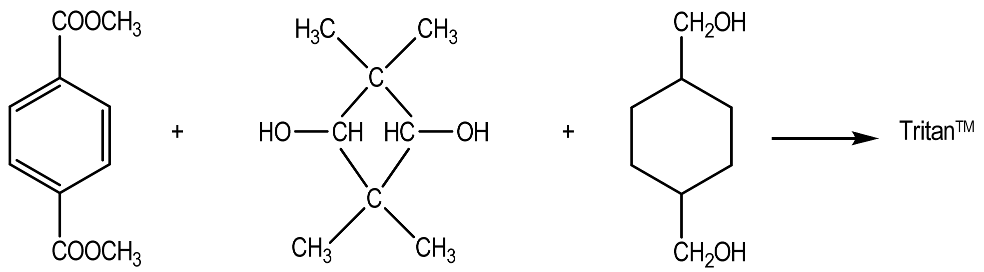
The second step in the polymerization sequence is the polycondensation of the oligomer. The reaction temperature must be above the melting point of the polymer and below the temperature at which decomposition occurs too rapidly. Production of the commercial product, the homopolymer polyethylene naphthalate (PEN) involves a solid state polymerization step.

The report includes process chemistry and technology descriptions along with pertinent flowsheets.

## Tritan™ Copolyester

Eastman Chemical markets a copolyester under the name Tritan™. Tritan™, introduced in 2007, is a polymer produced from dimethyl terephthalate, 1,4-cyclohexanedimethanol, and 2,2,4,4-tetramethyl-1,3-cyclobutanediol.




Dimethyl Terephthalate 2,2,4,4-tetramethyl-1,3-cyclobutanediol 1,4-cyclohexanedimethanol

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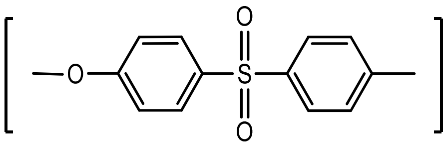
The process chemistry is detailed in the report, as well as a speculative process description with pertinent flow diagrams for the production of Tritan™ in a commercial size plant. Tritan's respective monomers are also discussed.

### Polyethersulfone

All sulfone-containing polymers contain two essential elements - the $SO_2$ group and an ether bridging -O- moiety. A range of polymers exist with these characteristics and are termed polysulfone, polyethersulfone, polyarylsulfone and polyphenylsulfone for example. However, two of the most common products on the market are polysulfone and polyethersulfone (PES).

The production synthesis of PES (whose repeating unit is shown below) is by nucleophilic substitution of 4,4′-dichlorodiphenyl sulfone (DCDPS) by 4,4′-dihydroxydiphenyl sulfone (DHDPS) in a dipolar aprotic solvent such as sulfolane, diphenyl sulfone or NMP.

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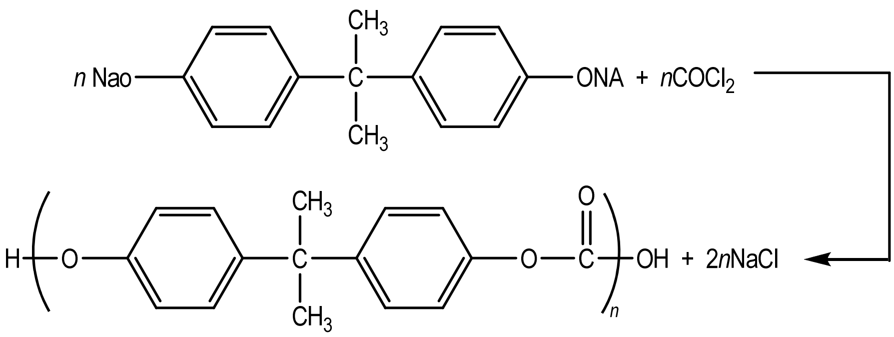
Conceptual process flow diagrams and descriptions for the production of polyethersulfone are presented in the report. The process consists of polymerization, polymer recovery, solvent recovery, and product handling systems.

### Polycarbonate

Until recently, Polycarbonate has conventionally been produced via several variations of the interfacial technology. In it, alkali salts of bisphenol A in aqueous solution are phosgenated in the presence of an inert solvent via the reaction below. The process chemistry is expanded upon in the report.

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Polycarbonate can also be produced via solution or melt processes, but only the melt transesterification process has found commercial viability in recent years, largely due to its environmental superiority.

There are several commercial incarnations of the interfacial technology. They are similar in overall concept, but there differences in several key areas. In the report, process description and pertinent flow diagrams are given which summarizes a well-practiced interfacial design for the production of polycarbonate.

## ECONOMICS

Several cases have been considered for the production of BPA-free resins and polycarbonate. Furthermore, production cost estimates have been generated for the production of raw materials used in the production of the polymers.

The selected cases are:

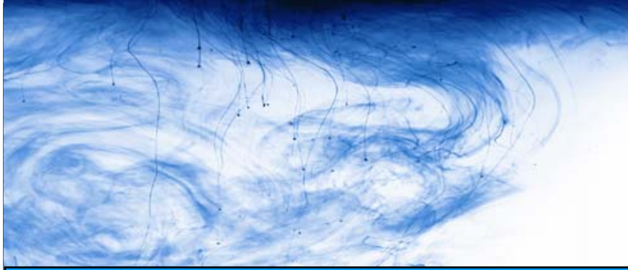
- HDPE Blow Molding (Slurry Process)
- Isotactic Metallocene Polypropylene (Homopolymer, Bulk Process)
- Polyethylene Naphthalate (Integrated Continuous MP + SS Process)
- Tritan$^{TM}$ (Melt + SSP Process)
- Polyethersulfone (Hydrolysis of DCDPS Process)
- Polycarbonate (Interfacial Process)

## SUPPLY OVERVIEW

This section provides a global supply overview for the resins mentioned in this report.

At the time of writing the plastic baby bottles industry is facing a number of challenges. These factors paint a rather challenging picture of the industry at least for the short to medium term. Some of the factors include:

- Health issues associated with BPA that continue to affect the market
- Competition from glass baby bottles
- Cost of production
- The stronger position in the supply chain of major retailers
- Development of new BPA-free resins.



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