

High Performance Polyesters (94/95S6)

Polyethylene terephthalate (PET) is a highly versatile polymer that is produced in large volume and used in a variety of end uses and physical forms. PET finds widespread application in blow molded containers for beverages and food, sheet and film for packaging, fiber for apparel, domestic and industrial uses, and engineering resins used in automobiles and appliances. The popularity of PET is based on its favorable balance of properties and price.

However, in certain end-use applications the properties of PET fall short of optimum and substitution, in part or wholly, of one or both of the monomers has led to polyesters with improved properties. Of course this substitution has economic implications. The objective of this report is to examine some of the newer, higher performing polyesters with a focus on the cost/performance issues. The polyesters investigated include:

- PET
- Acid modified (via isophthalic acid) PET
- Glycol modified (via cyclohexanedimethanol) PET
- UV resistant glycol modified PET
- Polyethylene naphthalate (PEN)
- Eight percent naphthalate/PET copolymer
- Polytrimethylene terephthalate

Homopolymer PET is made from terephthalic acid (PTA) and ethylene glycol (EG) as monomers. Higher performance PET copolymers are a result of substitution of other monomers for a portion of the acid or glycol component. This report includes PET copolymers in which isophthalic acid (IPA) is substituted for some of the terephthalic acid or cyclohexane dimethanol (CHDM) is substituted for some of the ethylene glycol. The resulting copolymers possess improved processability and performance including superior clarity of molded articles. The various uses of acid modified and glycol modified PET are discussed in the commercial section of this report.

Process technology used in the production of CHDM is presented with a detailed process flowsheet and description. Development of the estimated cost of CHDM production includes an estimate of the cost of the required dimethyl terephthalate feedstock. The production costs of terephthalic acid, isophthalic acid, and ethylene glycol also are estimated on a consistent basis. This input is then combined to yield estimates of PET homopolymer and PET copolymer production based on acid modification or glycol modification.

Polyethylene naphthalate (PEN) is a newly commercialized polyester, which, by virtue of its more rigid backbone based on naphthalene, offers higher performance than PET. There is across-the-board improvement when comparing PEN's properties to PET's, with

notable differences in temperature resistance, gas barrier properties, and UV light resistance. Since PEN is more costly than PET, it is especially fortuitous that small proportions of PEN, either as copolymers or blends, can impart significant property improvements to PET. The various applications for which naphthalate homopolymer or copolymers/blends are being considered are discussed in this report.

The monomers used in PEN production are dimethyl 2,6-naphthalene dicarboxylate (dimethyl 2,6-NDC) and ethylene glycol. Process technology used in dimethyl 2,6-NDC production, including a detailed process flowsheet and description, is provided. The estimated production cost for dimethyl 2,6-NDC is based, in turn, on an estimate of its precursor 2,6-dimethyl naphthalene's cost. The costs of PEN production are then estimated from those of dimethyl 2,6-NDC and EG.

Polytrimethylene terephthalate (PTT) is a polymer composed of terephthalic acid and trimethylene glycol (1,3-propanediol). This polymer has been known for many years, but commercialization was delayed by the lack of an economical route to 1,3-propanediol (1,3-PDO), an obstacle that has been overcome by a process using ethylene oxide and synthesis gas as feedstocks. An earlier route based on acrolein is still practiced.

A detailed process flowsheet and description of the production of 1,3-PDO is included in this report. The production cost is developed as an input to PTT's cost estimate.

PTT is initially targeted as a replacement for nylon 6 and 6,6 in fibers for carpets and textiles. In carpet fiber, PTT displays the resilience of nylon and the inherent stain resistance of PET. PTT fiber also can be disperse dyed at atmospheric boil without using a chemical carrier, an important environmental advantage that allows carpets made of PTT to be continuously dyed and printed. Other advantageous properties of PTT used in carpet manufacture are a class 1 flammability rating and low electrostatic propensity.