

# Terephthalic Acid

## Table of Contents

A Report by **NexantThinking™**

Process Evaluation/Research Planning (PERP) Program

PERP Report 2015-3– Published September 2015

[www.nexantthinking.com](http://www.nexantthinking.com)

Section	Page
1 Executive Summary .....	1
1.1 TECHNOLOGY .....	1
1.1.1 Value Chain .....	1
1.1.2 Chemistry .....	1
1.1.3 Basic Technology Offering .....	3
1.1.4 Licensors and Major Producers .....	4
1.1.5 Technology Developments .....	5
1.2 ECONOMICS .....	6
1.2.1 Process Comparison .....	6
1.2.2 Regional Comparison .....	7
1.2.3 Conclusions .....	8
1.3 COMMERCIAL .....	9
1.3.1 Business Developments .....	9
1.3.2 Applications .....	10
1.3.3 Markets .....	11
2 Introduction .....	15
2.1 VALUE CHAIN .....	15
2.2 OVERVIEW OF CHEMISTRY AND CONVENTIONAL TECHNOLOGY .....	16
2.2.1 Chemistry .....	16
2.2.2 Conventional Technology .....	17
2.3 PTA HAS BEEN AN EVOLVING TECHNOLOGY .....	21
2.4 LICENSORS AND MAJOR PRODUCERS .....	21
2.4.1 BP .....	22
2.4.2 Davy Process Technology/Dow (DPT/DOW) .....	22
2.4.3 Grupo Petrotex .....	22
2.4.4 GTC Technology .....	22
2.4.5 INVISTA Performance Technologies .....	23

2.5	BUSINESS DEVELOPMENTS .....	23
2.6	KEY PHYSICAL AND THERMODYNAMIC PROPERTIES .....	24
2.7	REGULATORY REQUIREMENTS .....	25
2.7.1	Health Hazards.....	25
2.7.2	Storage and Transportation .....	25
2.7.3	Regulatory .....	25
3	PTA Technology .....	26
3.1	CHEMISTRY .....	26
3.2	CONVENTIONAL PROCESS .....	27
3.2.1	CTA Production Process .....	31
3.2.2	PTA Production Process .....	34
3.3	DAVY PROCESS TECHNOLOGY/DOW (DPT/DOW) .....	37
3.3.1	CTA Production Process .....	38
3.3.2	PTA Production Process .....	40
3.3.3	Process Features .....	42
3.4	INVISTA.....	43
3.4.1	Oxidation Plant Process .....	44
3.4.2	Purification Plant Process .....	47
3.4.3	Process Features .....	49
3.5	BP .....	49
3.5.1	Process Description .....	50
3.5.2	Process Features .....	53
3.6	GTC TECHNOLOGY.....	54
3.6.1	Process Description .....	54
3.6.2	Process Performances .....	59
3.6.3	Process Features .....	62
3.7	GPT .....	63
3.7.1	GPT iPTA® Process .....	63
3.7.2	Process Features .....	69
3.8	DIFFERENT GRADES OF TEREPHTHALIC ACID.....	70
3.8.1	Medium Quality Terephthalic Acid .....	70
3.8.2	Quality and Color Formation .....	70
3.8.3	Application Comments .....	72
4	Developing Technology and Patents .....	74
4.1	PROCESS SIMPLIFICATION AND COST REDUCTION.....	74
4.1.1	Dow/Davy Process Technology: U.S. Patent 20150038737 A1 (February 5, 2015).....	74
4.1.2	Dow/Davy Process Technology: U.S. Patent 20130310602 A1 (November 21, 2013) .....	74
4.1.3	INVISTA: WO patent 2011100682 A2 (August 18, 2011).....	74

4.2	PURIFICATION WITHOUT HYDROGENATION .....	75
4.2.1	UOP: U.S. Patent 8754254 B2 (June 17, 2014) .....	75
4.2.2	Mitsubishi Gas Chemical: EP Patent 1389609 B1 (September 11, 2013) .....	75
4.3	ENERGY RECOVERY .....	76
4.3.1	Grupo Petrotemex: U.S. Patent 8236921 B1 (August 7, 2012) .....	76
4.3.2	BP: U.S. Patent 8,173,834 B2 (May 8, 2012) .....	76
4.4	PROCESS OPTIMIZATION .....	77
4.4.1	UOP: U.S. Patent 20140171679A1 (June 19, 2014) .....	77
4.5	ALTERNATIVE FEEDSTOCKS .....	77
4.5.1	UOP: WO patent 2013101334 A1 and 2013101332 A1 (July 4, 2013) .....	77
4.6	GREEN ROUTES TO PTA.....	78
4.6.1	Grupo Petrotemex: U.S. Patent 20120323039 A1 (December 20, 2012)...	78
4.6.2	UOP: U.S. Patent 8314267 B2 (November 20, 2012) .....	78
4.6.3	Micromidas: WO 2012170520 A1 (December 13, 2012).....	79
4.6.4	Amyris/Genomatica: U.S. Patent 20140302573 A1 (October 9, 2014).....	81
4.6.5	Anellotech: U.S. Patent 20090227823 A1 (September 10, 2009) .....	82
4.6.6	Gevo: U.S. Patent 20110087000 A1 (April 14, 2011) & U.S. Patent 8450543 B2 (May 28, 2013).....	83
4.6.7	Virent: U.S. Patent 20140349361 A1 (November 27, 2014).....	83
4.6.8	Stora: U.S. Patent 20130178650 A1 (July 11, 2013).....	84
5	Economics.....	86
5.1	COSTING BASIS .....	86
5.1.1	Investment Basis .....	86
5.1.2	Pricing Basis.....	86
5.1.3	Cost of Production Basis .....	87
5.2	PROCESS COMPETITIVENESS .....	88
5.2.1	Conventional PTA Production .....	88
5.2.2	COMPRESS PTA Production .....	90
5.2.3	INVISTA PTA Production .....	92
5.2.4	BP PTA Production .....	94
5.2.5	GTC Technology PTA Process .....	96
5.2.6	GPT PTA Production.....	98
5.2.7	Conclusion.....	100
5.3	REGIONAL COMPETITIVENESS .....	101
5.4	CONCLUSIONS .....	107
5.5	SENSITIVITY STUDY .....	108
5.5.1	<i>para</i> -Xylene Price.....	108
5.5.2	Plant Scale .....	109
6	Commercial Applications .....	110

6.1	FIBER .....	110
6.1.1	Textile Fibers .....	110
6.1.2	Carpet Facing .....	111
6.1.3	Industrial Fibers .....	111
6.2	CONTAINER .....	111
7	Regional Market Review .....	113
7.1	GLOBAL OVERVIEW .....	113
7.1.1	Consumption .....	113
7.1.2	Supply .....	114
7.1.3	Supply, Demand, and Trade .....	115
7.2	NORTH AMERICA .....	116
7.2.1	Consumption .....	116
7.2.2	Supply .....	117
7.2.3	Supply, Demand, and Trade .....	118
7.3	WESTERN EUROPE .....	120
7.3.1	Consumption .....	120
7.3.2	Supply .....	120
7.3.3	Supply, Demand, and Trade .....	122
7.4	ASIA PACIFIC .....	124
7.4.1	Consumption .....	124
7.4.2	Supply .....	125
7.4.3	Supply, Demand, and Trade .....	129
8	Glossary .....	130
9	References .....	132

<b>Appendix</b>		<b>Page</b>
A	Definitions of Capital Cost Terms Used in Process Economics.....	A-1
B	Definitions of Operating Cost Terms Used in Process Economics .....	B-1
C	PERP Program Title Index (2006 - 2015) .....	C-1

Figure	Page
1.1 Polyester Value Chain.....	1
1.2 Purified Terephthalic Acid Process Cost Comparison .....	7
1.3 Purified Terephthalic Acid Process Regional Cost Comparison.....	8
1.4 Global PTA Capacity Addition .....	13
1.5 Global PTA Capacity .....	13
2.1 Polyester Value Chain.....	15
2.2 Crude Terephthalic Acid Process (Block Flow Diagram) .....	18
2.3 Purified Terephthalic Acid Process .....	19
3.1 Crude Terephthalic Acid Process (Block Flow Diagram) .....	28
3.2 Purified Terephthalic Acid Process .....	29
3.3 Crude Terephthalic Acid Process Flow Diagram .....	32
3.4 Purified Terephthalic Acid Process Flow Diagram .....	35
3.5 COMPRESS™ PTA - CTA Flow Diagram .....	39
3.6 COMPRESS™ PTA - Purification Process Flow Diagram.....	41
3.7 INVISTA Oxidation Plant Process Flow Diagram.....	45
3.8 INVISTA Purification Plant Process Flow Diagram .....	48
3.9 BP Terephthalic Acid.....	51
3.10 GTC Technology Flow Diagram .....	55
3.11 GTC Technology Basic Process Diagram.....	56
3.12 Solubility Curve in NMP <sup>(4)</sup> .....	59
3.13 Solubility Curve in Methanol <sup>(4)</sup> .....	60
3.14 Water Ratio Influence on Conversion .....	61
3.15 Hydrogen Peroxide Ratio Influence on Conversion .....	61
3.16 GPT iPTA Block Flow Diagram .....	64
3.17 GPT iPTA Process Flow Diagram.....	65
4.1 Solubility of Terephthalic Acid and 4-CBA in Acetic Acid and Ionic Liquid Solvent <sup>(0)</sup> .....	75
4.2 Reaction Scheme for the Oxidation of p-toluic Acid.....	77
4.3 UOP's Green Route to PTA .....	79
4.4 Chemical Scheme of Biomass to Terephthalic Acid .....	80
4.5 Micromidas Process .....	81
4.6 Chemical Scheme of Muconic acid to PTA .....	81
4.7 Simplified Block Flow Diagram for Anellotech's Biomass to Aromatics™ Process .....	82
4.8 Chemical Scheme of Isobutanol to PTA .....	83
4.9 Mass Balance of <i>para</i> -Xylene Production <sup>(0)</sup> .....	84
4.10 Stora's Reaction Scheme.....	85
5.1 Purified Terephthalic Acid Process Cost Comparison .....	101
5.2 Purified Terephthalic Acid Process Regional Cost Comparison .....	106
5.3 Historical <i>para</i> -Xylene and Crude Oil Prices.....	108

5.4	Variation in Cost of Production.....	108
5.5	Variation in Cost of Production with Plant Scale .....	109
6.1	Fi-Cell Foamed PET Bottles.....	112
7.1	Global PTA Capacity Addition .....	115
7.2	Global PTA Capacity .....	115
7.3	End-use of PTA in North America-2015.....	117
7.4	North America PTA Supply/Demand and Trade .....	119
7.5	PTA end-use in Western Europe in 2015.....	120
7.6	Western Europe PTA Supply/ Demand and Trade .....	124
7.7	PTA End-use in Asia .....	125
7.8	Asia Pacific PTA Supply/Demand and Trade.....	129

<b>Table</b>	<b>Page</b>
1.1 Molar Efficiency of Terephthalic Acid Technology .....	3
1.2 Purified Terephthalic Acid Technology Licensors .....	4
1.3 Global PTA Consumption by Region .....	12
2.1 Purified Terephthalic Acid Technology Licensors .....	21
2.2 Typical PTA Specifications.....	24
3.1 Molar Efficiency of Terephthalic Acid Technology .....	31
3.2 Characteristics of PTA.....	36
3.3 Required Raw Material Characteristics .....	37
3.4 Typical Purification by Solvent Crystallization Efficiency .....	62
3.5 Comparison of PTA and MTA Specifications .....	71
5.1 Pricing Basis for Terephthalic Acid .....	87
5.2 Cost of Production for Purified Terephthalic Acid Process: Oxidation/Hydrogenation (Conventional) .....	89
5.3 Cost of Production for Purified Terephthalic Acid Process: Oxidation/Hydrogenation (COMPRESS).....	91
5.4 Cost of Production for Purified Terephthalic Acid Process: Oxidation/Hydrogenation (INVISTA P8).....	93
5.5 Cost of Production for Purified Terephthalic Acid Process: Oxidation/Hydrogenation (BP) .....	95
5.6 Cost of Production for Purified Terephthalic Acid Process: Oxidation/Hydrogenation (GTC).....	97
5.7 Cost of Production for Purified Terephthalic Acid Process: Dual Oxidation/No Hydrogenation (GPT).....	99
5.8 Purified Terephthalic Acid Process Cost Comparison .....	100
5.9 Cost of Production for Purified Terephthalic Acid (Licensor: BP, China, first quarter, 2015) .....	102
5.10 Cost of Production for Purified Terephthalic Acid (Licensor: INVISTA, China, first quarter, 2015).....	103
5.11 Cost of Production for Purified Terephthalic Acid (Licensor: GPT, China, first quarter, 2015) .....	104
5.12 Cost of Production for Purified Terephthalic Acid (Licensor: BP, Western Europe, first quarter, 2015) .....	105
5.13 Purified Terephthalic Acid Process Regional Cost Comparison .....	106
7.1 Global PTA Consumption by Region .....	114
7.2 Global PTA Supply/Demand and Trade .....	116
7.3 North America PTA Capacity .....	118
7.4 North America PTA Supply/Demand and Trade .....	119
7.5 PTA Plants in Western Europe.....	122
7.6 Western Europe PTA Supply/ Demand and Trade .....	123
7.7 PTA Capacity in Asia.....	126
7.8 Asia Pacific PTA Supply/Demand and Trade.....	129

# Nexant Thinking™

## Process Evaluation/Research Planning



The NexantThinking™ Process Evaluation/Research Planning (PERP) program is recognized globally as the industry standard source for information relevant to the chemical process and refining industries. PERP reports are available as a subscription program or on a single report basis.

### Contact Details:

**New York:** Marcos Nogueira Cesar, Vice President, Global Products, E&CA: Nexant Thinking™  
Phone: + 1-914-609-0324, e-mail: [mcesar@nexant.com](mailto:mcesar@nexant.com)

**New York:** Heidi Junker Coleman, Global Programs Support Manager  
Phone: + 1-914-609-0381, e-mail: [hcoleman@nexant.com](mailto:hcoleman@nexant.com)

Nexant, Inc. ([www.nexant.com](http://www.nexant.com)) is a leading management consultancy to the global energy, chemical, and related industries. For over 38 years, Nexant has helped clients increase business value through assistance in all aspects of business strategy, including business intelligence, project feasibility and implementation, operational improvement, portfolio planning, and growth through M&A activities. Nexant has its main offices in San Francisco (California), White Plains (New York), and London (UK), and satellite offices worldwide.

Copyright © by Nexant Inc. 2015. All Rights Reserved.