

1,4-Butanediol/Tetrahydrofuran

Table of Contents

A Report by **NexantThinking™**

Process Evaluation/Research Planning (PERP) Program

PERP Report 2017-4 – Published November 2017

www.nexantthinking.com

Section	Page
1 Executive Summary	1
1.1 TECHNOLOGY LICENSING STATUS	2
1.2 TECHNOLOGY REVIEW.....	2
1.3 PROCESS ECONOMICS	3
1.3.1 Process Benchmarking.....	3
1.3.2 Regional Process Economics Comparison at Existing BDO Plant Capacities	5
1.3.3 Regional Process Economics Comparison at 100 Thousand Tons per Year BDO Capacity	6
1.4 COMMERCIAL ANALYSIS.....	6
1.4.1 1,4-Butanediol Market Analysis.....	6
1.4.2 Tetrahydrofuran Market Analysis	7
2 Introduction.....	8
2.1 TECHNOLOGY OVERVIEW – HISTORICAL DEVELOPMENT	9
2.1.1 Acetylene-Based Technology (1930s – 1970s).....	9
2.1.2 Beyond Acetylene-Based Production (1970s – 1990s)	12
2.1.3 Commoditization of BDO, THF, and Other Derivatives (2000 – Present)	14
2.1.4 Emergence of Bio-Based Routes (Late 2000s – Present)	14
2.2 BUSINESS DEVELOPMENTS.....	14
2.2.1 Current State of Mature Technologies	15
2.2.2 Emerging Technologies and Innovation	18
2.3 TECHNOLOGY HOLDERS AND LICENSING STATUS	21
2.4 STRATEGIC AND BUSINESS CONSIDERATIONS.....	21
2.5 PHYSICAL AND THERMODYNAMIC PROPERTIES.....	23
2.6 SPECIFICATIONS	23
2.7 HEALTH HAZARDS.....	24
2.7.1 1,4-Butanediol.....	24
2.7.2 Tetrahydrofuran	24
2.8 STORAGE AND TRANSPORTATION.....	24

2.8.1	1,4 Butanediol	24
2.8.2	Tetrahydrofuran	25
3	Commercial Technologies	26
3.1	PROCESSES FOR 1,4-BUTANEDIOL	26
3.1.1	Reppe Process – Acetylene-Based Route	27
3.1.2	Maleic Anhydride Based Route – Johnson Matthey Davy Technologies	40
3.1.3	Dairen Propylene (via Allyl Alcohol) Route	47
3.1.4	Geminox® from <i>n</i> -Butane via Maleic Acid (Ashland)	50
3.1.5	LyondellBasell Propylene Oxide Route	56
3.1.6	Mitsubishi Chemical Corporation Butadiene Acetoxylation.....	66
3.2	PROCESSES FOR TETRAHYDROFURAN.....	72
3.2.1	Conventional Dehydration of 1,4-Butanediol	72
3.2.2	Mitsubishi Chemical Butadiene Acetoxylation	78
4	Patent Developments.....	80
4.1	INTRODUCTION.....	80
4.2	DEVELOPMENTS BY BASF	82
4.3	DEVELOPMENTS BY MITSUBISHI	83
4.4	DEVELOPMENTS BY DAIREN CHEMICAL CORPORATION.....	84
4.5	DEVELOPMENTS BY ASHLAND	84
4.6	DEVELOPMENTS BY INVISTA	84
4.7	DEVELOPMENTS BY JOHNSON MATTHEY DAVY TECHNOLOGIES (JM DAVY)	85
4.8	DEVELOPMENTS BY CHINESE PRODUCERS	85
5	Process Economics	87
5.1	COSTING BASIS	87
5.2	INVESTMENT BASIS	87
5.3	PRICING BASIS.....	87
5.4	COST OF PRODUCTION BASIS.....	89
5.5	TECHNO-ECONOMICS FOR CONVENTIONAL 1,4-BUTANEDIOL PROCESSES	89
5.5.1	Cost of Producing BDO from Acetylene - INVISTA™ Process.....	90
5.5.2	Cost of Producing BDO from Acetylene Conventional Reppe Process	94
5.5.3	Cost of Producing BDO via JM Davy Maleic Anhydride Process	98
5.5.4	Cost of Producing BDO via the Allyl Alcohol Process	100
5.5.5	Cost of Producing BDO via the Propylene Oxide Process	102
5.5.6	Cost of Producing BDO from Butadiene	104
5.5.7	Cost of Producing BDO from <i>n</i> -Butane via Maleic Acid (Geminox® Process)	106
5.6	COMPARISON OF PROCESSES TO PRODUCE 1,4-BUTANEDIOL	108
5.6.1	Regional Comparison of 1,4-Butanediol Routes at Capacities of Existing Plants	108
5.6.2	Regional comparison of 1,4-Butanediol Routes at 100 00 Ton per Year Plant Capacity	109

5.7	SENSITIVITY ANALYSIS	110
5.7.1	Feedstock Price Sensitivity.....	110
5.8	TECHNO-ECONOMICS FOR TETRAHYDROFURAN	111
5.8.1	Dehydration of 1,4-Butanediol.....	111
6	1,4-Butanediol Tetrahydrofuran End-Use Analysis	114
6.1	TETRAHYDROFURAN (THF)	115
6.1.1	THF as a Resin Solvent.....	116
6.1.2	THF as a Reaction Solvent or Starting Material	117
6.2	POLYBUTYLENE TEREPHTHALATE (PBT)	119
6.2.1	Properties of PBT	119
6.2.2	Industrial Applications of PBT	120
6.2.3	Developments in PBT Products	122
6.3	GAMMA-BUTYROLACTONE (GBL)	122
6.3.1	<i>n</i> -Methyl Pyrrolidone (NMP)	123
6.3.2	2-Pyrrolidone.....	123
6.3.3	<i>N</i> -Vinyl Pyrrolidone (NVP)	123
6.4	POLYURETHANE THERMOPLASTIC ELASTOMERS AND FIBERS	124
6.4.1	Thermoplastic Polyurethanes.....	124
6.4.2	Castable Polyurethanes	125
6.4.3	Reaction Injection Molding	126
6.5	COPOLYESTER-ETHER THERMOPLASTIC ELASTOMERS	127
7	1,4-Butanediol Regional Market Analysis	128
7.1	GLOBAL OVERVIEW	128
7.1.1	Demand.....	128
7.1.2	Supply	130
7.1.3	Supply, Demand, and Trade	131
7.2	NORTH AMERICA	132
7.2.1	Demand.....	132
7.2.2	Supply	133
7.2.3	Supply, Demand, and Trade	133
7.3	WESTERN EUROPE	135
7.3.1	Demand.....	135
7.3.2	Supply	135
7.3.3	Supply, Demand, and Trade	136
7.4	ASIA PACIFIC (EXCL. CHINA)	137
7.4.1	Demand.....	137
7.4.2	Supply	137
7.4.3	Supply, Demand, and Trade	138
7.5	CHINA.....	139
7.5.1	Demand.....	139
7.5.2	Supply	140
7.5.3	Supply, Demand, and Trade	142

7.6	REST OF THE WORLD (ROW)	143
7.6.1	Demand.....	143
7.6.2	Supply	143
7.6.3	Supply, Demand, and Trade	144
8	Tetrahydrofuran Regional Market Analysis.....	145
8.1	GLOBAL	145
8.1.1	Demand.....	145
8.1.2	Supply	146
8.1.3	Supply, Demand, and Trade	147
8.2	NORTH AMERICA	148
8.2.1	Demand.....	148
8.2.2	Supply	148
8.2.3	Supply, Demand, and Trade	149
8.3	WESTERN EUROPE	150
8.3.1	Demand.....	150
8.3.2	Supply	150
8.3.3	Supply, Demand, and Trade	151
8.4	ASIA PACIFIC (EXCL. CHINA)	152
8.4.1	Demand.....	152
8.4.2	Supply	152
8.4.3	Supply, Demand, and Trade	153
8.5	CHINA.....	154
8.5.1	Demand.....	154
8.5.2	Supply	154
8.5.3	Supply, Demand, and Trade	155
8.6	REST OF THE WORLD (ROW)	157
8.6.1	Demand.....	157
8.6.2	Supply	157
8.6.3	Supply, Demand, and Trade	157
9	Glossary	159
10	References	161

Appendix	Page
A COPS	A-1
B Definitions of Capital Cost Terms Used in Process Economics.....	B-1
C Definitions of Operating Cost Terms Used in Process Economics	C-1
D PERP Program Title Index (2006-2017)	D-1

Figure	Page
1.1 Evolution of BDO Technology Share by Feedstock	1
1.2 Percentages of Patents Granted by Region and Assignees	3
1.3 BDO Process Comparison (on Existing BDO plants' Capacity Basis).....	4
1.4 BDO Process Comparison (on 100 000 Ton per Year Plant Basis)	5
1.5 Global BDO Supply and Demand	6
1.6 Global Tetrahydrofuran Supply and Demand.....	7
2.1 Global Capacity Development by Process Technology	8
2.2 BDO/THF Technology and Global Capacity Timeline (1930s – 2000)	10
2.3 BDO/THF Technology and Global Capacity Timeline (2000s – to Date).....	11
2.4 Licensors Global BDO Market Share Evolution in 2012-2017	15
3.1 Evolution of BDO Technology Share by Feedstock.....	26
3.2 Acetylene Technology Share by Licensor and by Region	27
3.3 Synthesis of 1,4-Butynediol from Acetylene and Formaldehyde	31
3.4 Hydrogenation of 1,4 Butynediol to 1,4-Butanediol.....	33
3.5 INVISTA™ Simplified 1,4-Butanediol Process Schematic	35
3.6 INVISTA™ Synthesis of 1,4-Butynediol from Acetylene and Formaldehyde.....	36
3.7 INVISTA™ Hydrogenation of 1,4-Butynediol to 1,4-Butanediol.....	37
3.8 DAVY™ BDO Process Maleic Anhydride Esterification and Hydrogenation	43
3.9 DAVY™ BDO Process Separation and Purification.....	45
3.10 Allyl Alcohol via Propylene Acetoxylation and Hydrolysis	48
3.11 Geminox® Maleic Acid Production.....	53
3.12 Geminox® Maleic Acid Hydrogenation	55
3.13 Propylene Oxide Isomerization to Allyl Alcohol.....	59
3.14 4-Hydroxybutyraldehyde via Allyl Alcohol Hydroformylation	62
3.15 1,4-Butanediol via 4-Hydroxybutyraldehyde Hydrogenation.....	64
3.16 1,4-Diacetoxybutene Production via Butadiene Acetoxylation.....	69
3.17 1,4-Butanediol from 1,4-Diacetoxybutene via Hydrogenation and Hydrolysis	71
3.18 BDO Hydrogenation to THF	73

3.19	Ashland: BDO Hydrogenation to THF	75
3.20	INVISTA™: BDO Hydrogenation to THF	77
3.21	Mitsubishi: THF from 1,4-Diacetoxybutene	79
4.1	Overall Patent Activity by the Year	80
4.2	Percentages of Patents Granted by Region and Assignees	81
5.1	Regional BDO Cost of Production Comparison (on Existing BDO Plants' Capacity Basis) ..	108
5.2	Regional BDO Cost of Production Comparison (on 100 000 Ton per Year Plant Basis)	109
5.3	BDO Production Cost Sensitivity to Feedstock Cost	110
6.1	1,4-Butanediol Value Chain.....	114
7.1	Global BDO End-Use	128
7.2	Global Breakdown of BDO Consumption.....	129
7.3	Global BDO Capacity by Region	130
7.4	Global BDO Supply and Demand	132
7.5	North America BDO End-Use.....	132
7.6	North America BDO Supply and Demand.....	134
7.7	Western Europe BDO End-Use.....	135
7.8	Western Europe BDO Supply and Demand.....	136
7.9	Asia Pacific (excluding China) BDO End-Uses	137
7.10	Asia Pacific (excluding China) BDO Supply and Demand	139
7.11	China BDO End-Use	139
7.12	China BDO Supply and Demand.....	142
7.13	Rest of the World BDO End-Uses	143
7.14	Rest of the World BDO Supply and Demand	144
8.1	Global Breakdown of THF Consumption.....	145
8.2	Global THF Capacity by Region.....	146
8.3	Global THF Supply and Demand	147
8.4	North America THF Supply and Demand.....	149
8.5	Western Europe THF Supply and Demand.....	151
8.6	Asia Pacific (excluding China) THF Supply and Demand	153
8.7	China THF Supply and Demand	156
8.8	Rest of the World THF Supply and Demand.....	158

Table	Page
1.1 Conventional Technology Holders and Licensors	2
2.1 Conventional Technology Holders and Licensors	21
2.2 Strategic/Business Considerations	22
2.3 Key Physical and Thermodynamic Properties of BDO	23
2.4 Key Physical and Thermodynamic Properties of THF	23
2.5 Typical Commercial Specification for BDO	23
2.6 Typical Commercial Specification for THF	24
4.1 Patents Granted to BASF	82
4.2 Patents Granted to Mitsubishi	83
4.3 Patents Granted to Dairen	84
4.4 Patents Granted to Ashland	84
4.5 Patents Granted to INVISTA	85
4.6 Patents Granted to JM Davy	85
4.7 Patents Granted to Sinopec	86
4.8 Patents Granted to Xinjiang Markor Chemical	86
4.9 Patents Granted to Inner Mongolia Dongyuan Technology	86
5.1 Pricing Basis for Raw Materials, Utilities and Labor	88
5.2 Cost of Production Estimate: 1,4-Butanediol Process: Reppe Chemistry followed by Hydrogenation of Acetylene (ex-POx), Region: USGC	91
5.3 Cost of Production Estimate: 1,4-Butanediol Process: Reppe Chemistry followed by Hydrogenation of Acetylene (ex- CaC ₂), Region: China	93
5.4 Cost of Production Estimate: 1,4-Butanediol Process: Reppe Chemistry followed by Hydrogenation of Acetylene, Region: USGC	95
5.5 Cost of Production Estimate: 1,4-Butanediol Process: Reppe Chemistry followed by Hydrogenation of Acetylene, Region: Western Europe	97
5.6 Cost of Production Estimate: 1,4-Butanediol Process: DPT Maleic Anhydride Hydrogenation, 4:1 BDO to THF Output, Region: China	99
5.7 Cost of Production Estimate: 1,4-Butanediol Process: Hydroformylation of Allyl Alcohol, Region: China	101
5.8 Cost of Production Estimate: 1,4-Butanediol Process: Propylene Oxide Isomerization and Hydroformylation, Region: USGC	103
5.9 Cost of Production Estimate: 1,4-Butanediol Process: Butadiene Acetoxylation, Region: Taiwan	105

5.10	Cost of Production Estimate: 1,4-Butanediol Process: Hydrogenation of Maleic Acid Via Butane Oxidation, Region: USGC	107
5.11	Cost of Production Estimate for THF Process: Dehydration of 1,4-Butanediol, Region USGC	112
5.12	Cost of Production Estimate for THF Process: Dehydration of 1,4-Butanediol, Region China.....	113
6.1	GBL and Derivatives Applications	122
7.1	Global BDO Consumption by Region.....	129
7.2	Global BDO Supply and Demand	131
7.3	North America BDO Capacity.....	133
7.4	North America BDO Supply and Demand.....	134
7.5	Western Europe BDO Capacity.....	135
7.6	Western Europe BDO Supply and Demand.....	136
7.7	Asia Pacific (excluding China) BDO Capacity.....	138
7.8	Asia Pacific (excluding China) BDO Supply and Demand	138
7.9	China BDO Capacity	141
7.10	China BDO Supply and Demand.....	142
7.11	Rest of the World BDO Capacity.....	143
7.12	Rest of the World BDO Supply and Demand	144
8.1	Global THF Consumption by Region	146
8.2	Global THF Supply and Demand	147
8.3	North America THF Capacity	148
8.4	North America THF Supply and Demand.....	149
8.5	Western Europe THF Capacity	150
8.6	Western Europe THF Supply and Demand.....	151
8.7	Asia Pacific (excluding China) BDO Capacity.....	152
8.8	Asia Pacific (excluding China) THF Supply and Demand	153
8.9	China THF Capacity	155
8.10	China THF Supply and Demand	156
8.11	Rest of the World THF Capacity.....	157
8.12	Rest of the World THF Supply and Demand.....	157

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:

Americas:

Marcos Nogueira Cesar, Vice President, Global Products, E&CA: Nexant Thinking™
Phone: + 1-914-609-0324, e-mail: mcesar@nexant.com

Erica Hill, Client Services Coordinator, E&CA-Products
Phone: + 1-914-609-0386, e-mail: ehill@nexant.com

EMEA:

Anna Ibbotson, Director, NexantThinking
Phone: +44-207-950-1528, aibbotson@nexant.com

Asia:

Chommanad Thammanayakatip, Managing Consultant, Energy & Chemicals Advisory
Phone: +66-2793-4606, email: chommanadt@nexant.com

Nexant, Inc. (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. 2017. All Rights Reserved.