

Oxo-Alcohols

Table of Contents

A Report by **NexantThinking™**

Process Evaluation/Research Planning (PERP) Program

PERP Report 2016-1 – Published July 2016

www.nexantthinking.com

Section	Page
1 Executive Summary	1
1.1 INTRODUCTION.....	1
1.2 COMMERCIAL TECHNOLOGIES	2
1.3 DEVELOPING TECHNOLOGIES	3
1.4 PROCESS ECONOMICS.....	4
1.5 GLOBAL MARKET ANALYSIS	5
1.6 STRATEGIC OUTLOOK FOR OXO ALCOHOLS.....	7
2 Introduction.....	8
2.1 OVERVIEW	8
2.2 PRODUCTION TECHNOLOGY.....	9
2.3 BUSINESS DEVELOPMENTS	10
2.4 TECHNOLOGY LICENSING STATUS AND MAJOR PRODUCERS	11
2.5 MAJOR DRIVERS AND END-USAGES	11
2.6 PHYSICAL AND THERMODYNAMIC PROPERTIES	12
2.7 SPECIFICATIONS	13
2.8 HEALTH HAZARDS	14
2.9 STORAGE AND TRANSPORTATION.....	14
3 Commercial Technologies.....	15
3.1 BACKGROUND AND CHEMISTRY.....	15
3.1.1 Introduction.....	15
3.1.2 Process Chemistry	16
3.1.3 Separation Processes	27
3.2 COMMERCIAL TECHNOLOGIES FOR CONVERSION OF PROPYLENE TO BUTYRALDEHYDES	28
3.2.1 JM's DAVY™/Dow LP Oxo Process	28
3.2.2 JM's DAVY™/Dow High Selectivity LP Oxo Process	30
3.2.3 Eastman Oxo Low Pressure Technology.....	32
3.2.4 Rhône-Poulenc/Ruhrchemie Process	34

3.2.5	BASF Process	36
3.2.6	Mitsubishi Process	37
3.2.7	Other Technologies	39
3.3	DOWNSTREAM PROCESSING OF BUTYRALDEHYDES TO OXO ALCOHOLS	39
3.3.1	Hydrogenation	39
3.3.2	Aldol Condensation and Hydrogenation.....	41
3.4	COMMERCIAL TECHNOLOGIES FOR CONVERSION OF MEDIUM CHAIN OLEFINS	45
3.4.1	Johnson Matthey Oxo Alcohols Process.....	45
4	Developing Technologies	49
4.1	RECENT DEVELOPMENTS IN HYDROFORMYLATION PROCESS TECHNOLOGY	49
4.1.1	Aldol Condensation Reactors.....	49
4.1.2	Purge System Recovery	49
4.1.3	Phosphite Catalyst Degradation Product Scrubbing Systems	50
4.1.4	Operational Improvements	51
4.2	RECENT DEVELOPMENTS IN HYDROFORMYLATION CATALYSTS.....	51
4.2.1	Developments that Increase Process <i>n/i</i> Ratio Flexibility	51
4.2.2	Developments in Catalysts for High Iso-Aldehyde Selectivity.....	52
4.2.3	Other Catalysts.....	54
4.3	RECENT DEVELOPMENTS IN BIO-BASED PRODUCTION OF TRADITIONAL OXO ALCOHOLS	54
4.3.1	Fermentation-Based Production	54
4.3.2	Bio-Based Synthetic Oxo Alcohols.....	55
5	Economics	57
5.1	COSTING BASIS	57
5.1.1	Investment Basis	57
5.1.2	Pricing Basis.....	57
5.1.3	Cost of Production Basis	59
5.2	PROCESS COMPETITIVENESS	59
5.2.1	DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 10 Process	60
5.2.2	DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 30 Process	62
5.2.3	DAVY/Dow 2-Ethylhexanol LP Oxo Selector 10 Process	64
5.2.4	DAVY/Dow 2-Ethylhexanol LP Oxo SM Selector 30 Process	66
5.2.5	DAVY/Dow 2-Propylheptanol LP Oxo SM Process	68
5.2.6	Johnson Matthey Isononanol Process	70
5.2.7	Summary	72
5.3	REGIONAL COMPETITIVENESS	75
5.3.1	DAVY/Dow <i>n</i> -Butanol LP Oxo SM Selector 10 Process	75

5.3.2	DAVY/Dow n-Butanol LP Oxo Selector 30 Process	79
5.3.3	DAVY/Dow 2-Ethylhexanol LP Oxo SM Selector 10 Process	83
5.3.4	DAVY/Dow 2-Ethylhexanol LP Oxo SM Selector 30 Process	87
5.3.5	DAVY/Dow 2-Propylheptanol LP Oxo SM Process	91
5.3.6	Johnson Matthey Isononanol Process	95
5.4	SENSITIVITY STUDY	98
5.4.1	<i>n</i> -Butanol Production Processes	98
5.4.2	2-Ethylhexanol Production Processes	99
5.4.3	DAVY/Dow 2-Propylheptanol LP Oxo SM Process	100
5.4.4	Johnson Matthey Isononanol Process	101
6	Global Markets	102
6.1	<i>N</i> -BUTANOL	103
6.1.1	Global	103
6.1.2	North America	106
6.1.3	Western Europe	108
6.1.4	Asia Pacific	111
6.2	ISOBUTANOL	117
6.2.1	Global	117
6.2.2	North America	120
6.2.3	Western Europe	122
6.2.4	Asia Pacific	124
6.3	2-ETHYLHEXANOL	128
6.3.1	Global	128
6.3.2	North America	130
6.3.3	Western Europe	133
6.3.4	Asia Pacific	136
7	Strategic Analysis	142
7.1	MARKET OUTLOOK	142
7.1.1	Outlook for <i>n</i> -Butanol and Isobutanol	142
7.1.2	Outlook for 2-Ethylhexanol	142
7.2	TECHNOLOGY OUTLOOK	147
7.2.1	Outlook for Conventional Technologies	147
7.2.2	Outlook for Developing Technologies	147
8	Glossary	149
9	References	150

Appendix	Page
A Additional Cost of Production Estimates	A-1
B PERP Program Title Index (2007 - 2016)	B-1

Figure	Page
1.1 Common Oxo Alcohols.....	1
1.2 Global <i>n</i> -Butanol Supply, Demand, and Trade	6
1.3 Global Isobutanol Supply, Demand, and Trade	6
1.4 Global 2-Ethylhexanol Supply, Demand, and Trade	7
2.1 Common Oxo Alcohols.....	8
3.1 Summary Reaction Equations for Oxo Reaction.....	16
3.2 Cobalt Tetracarbonyl Hydride.....	17
3.3 Insertion of Asymmetric Olefin into Cobalt Complex.....	18
3.4 Major Reactions of Acylcobalt Complexes in Oxo Reaction	19
3.5 Phosphine and Phosphite Ligands.....	20
3.6 Hydroformylation Reaction Mechanism for High Selectivity to the Linear Aldehyde	21
3.7 Example Phosphine and Phosphite Ligands.....	24
3.8 Bisphosphite Rhodium Complex	25
3.9 Effect of Ligands on Reaction Rate and Linearity	26
3.10 Hydroformylation of a Raffinate-2 (Mixed Butenes) Stream	27
3.11 DAVY™/Dow LP Oxo SM Selector SM 10 Process	29
3.12 DAVY™/Dow Oxo SM Selector SM 30 Process.....	31
3.13 BISBI Bisphosphite Ligand.....	33
3.14 Rhône-Poulenc/Ruhrchemie Process Scheme.....	35
3.15 Mitsubishi Process Scheme	38
3.16 Hydrogenation Process for <i>n</i> -/ <i>i</i> -butanol Production	40
3.17 2-EH Production via Aldolization of <i>n</i> -butanal and Hydrogenation of 2-Ethyl-2 Hexanal	42
3.18 2-Propylheptanol Aldol Process and Hydrogenation Sections.....	44
3.19 Johnson Matthey Oxo Alcohols Process.....	46
4.1 Dow Chemical Calixarene Bisphosphite and Triphenylphosphite Two-Ligand System.....	52
4.2 Eastman High Iso-Selectivity Catalyst Complex	53
5.1 <i>n</i> -Butanol Process Comparison.....	73
5.2 2-Ethylhexanol Process Comparison	74
5.3 Regional Cost Competitiveness for DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 10 Process.....	76
5.4 Regional Cost Competitiveness for DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 30 Process	79
5.5 Regional Cost Competitiveness for DAVY/Dow 2-Ethylhexanol LP Oxo Selector 10 Process.....	83
5.6 Regional Cost Competitiveness for DAVY/Dow 2-Ethylhexanol LP Oxo Selector 30 Process.....	87
5.7 Regional Cost Competitiveness for DAVY/Dow 2-Propylheptanol LP Oxo Process	91
5.8 Regional Cost Competitiveness for Johnson Matthey Isononanol Process	95
5.9 Sensitivity of <i>n</i> -Butanol Costs to Propylene Price Movements	98
5.10 Sensitivity of <i>n</i> -Butanol Costs to Capital Cost.....	99

5.11	Sensitivity of 2-Ethylhexanol Costs to Propylene Price Movements.....	99
5.12	Sensitivity of 2-Ethylhexanol Costs to Capital Costs.....	100
5.13	Sensitivity of 2-Propylheptanol Cost to Production Inputs-DAVY/ Dow 2-Propylheptanol LP Oxo Process	100
5.14	Sensitivity of Isononanol Cost to Production Inputs – Johnson Matthey Process	101
6.1	Global <i>n</i> -Butanol Consumption by End-Use, 2015	103
6.2	Global <i>n</i> -Butanol Capacity by Marketer, 2015	104
6.3	Global <i>n</i> -Butanol Supply, Demand, and Trade	105
6.4	North America <i>n</i> -Butanol Consumption, 2015.....	106
6.5	North America <i>n</i> -Butanol Supply, Demand, and Trade.....	108
6.6	Western Europe <i>n</i> -Butanol Consumption, 2015.....	109
6.7	Western Europe <i>n</i> -Butanol Supply, Demand, and Trade.....	110
6.8	Asia Pacific <i>n</i> -Butanol Consumption, 2015	113
6.9	Asia Pacific <i>n</i> -Butanol Supply, Demand, and Trade	116
6.10	Global Isobutanol Consumption by End-Use, 2015	118
6.11	Global Isobutanol Capacity by Marketer, 2015	119
6.12	Global Isobutanol Supply, Demand, and Trade	120
6.13	North America Isobutanol Consumption, 2015	121
6.14	North America Isobutanol Supply, Demand, and Trade	122
6.15	Western Europe Isobutanol Consumption, 2015	123
6.16	Western Europe <i>i</i> -Butanol Supply, Demand, and Trade	124
6.17	Asia Pacific Isobutanol Consumption, 2015	125
6.18	Asia Pacific Isobutanol Supply, Demand, and Trade	127
6.19	Global 2-Ethylhexanol Consumption by End-Use, 2015	128
6.20	Global 2-Ethylhexanol Capacity by Marketer in 2015	129
6.21	Global 2-Ethylhexanol Supply, Demand, and Trade	130
6.22	North America 2-Ethylhexanol Consumption by End-Use	131
6.23	North America 2-Ethylhexanol Supply, Demand, and Trade	132
6.24	Western Europe 2-Ethylhexanol Consumption by End-Use, 2015	134
6.25	Western Europe 2-Ethylhexanol Supply, Demand, and Trade	135
6.26	Asia Pacific 2-Ethylhexanol Consumption, 2015.....	138
6.27	Asia Pacific 2-Ethylhexanol Supply, Demand, and Trade	141

Table	Page
1.1 Bio-Oxo Alcohols Process Development	3
1.2 Recent Developments in Oxo Alcohols Technology	4
1.3 Summary of Oxo Alcohols Process Economics	5
1.4 Summary of Strategic Outlook for Oxo Alcohols	7
2.1 Characteristic Properties of <i>n</i> -Butanol, 2-Ethylhexanol, and 2-Propylheptanol	12
2.2 <i>n</i> -Butanol Commercial Specification	13
2.3 2-Ethylhexanol Commercial Specification.....	13
2.4 2-Propylheptanol Commercial Specification	13
3.1 Hydroformylation Catalysts	17
3.2 Typical LP Oxo SM SELECTOR SM 10 Process Characteristics	30
3.3 Comparison of DAVY™/Dow LP Oxo Processes	32
3.4 Comparison of LP Oxo Processes	33
3.5 Rhône-Poulenc/Ruhrchemie Process Characteristics	36
3.6 Typical BASF Process Characteristics.....	37
5.1 Pricing Basis for Oxo Alcohols	58
5.2 Cost of Production for: <i>n</i> -Butanol Process: DAVY/Dow LP Oxo Selector 10 Process	61
5.3 Cost of Production for: <i>n</i> -Butanol Process: DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 30 Process	63
5.4 Cost of Production Estimate for: 2-Ethylhexanol Process: DAVY/Dow 2-Ethylhexanol LP Oxo Selector 10 Process	65
5.5 Cost of Production Estimate for: 2-Ethylhexanol Process: DAVY/Dow 2-Ethylhexanol LP Oxo Selector 30 Process	67
5.6 Cost of Production Estimate for: 2-Propylheptanol Process: DAVY/Dow 2-Propylheptanol LP Oxo Process	69
5.7 Cost of Production Estimate for: Isononanol Process: Johnson Matthey	71
5.8 Summary of <i>n</i> -Butanol Process Economics.....	72
5.9 Summary of 2-Ethylhexanol Process Economics	74
5.10 Summary of Regional Cost Competitiveness for DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 10 Process.....	75
5.11 Cost of Production Estimate for: <i>n</i> -Butanol in Western Europe Process: DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 10 Process	77
5.12 Cost of Production Estimate for: <i>n</i> -Butanol in China Process: DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 10 Process	78
5.13 Summary of Regional Cost Competitiveness for DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 30 Process.....	79
5.14 Cost of Production Estimate for: <i>n</i> -Butanol in Western Europe Process: DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 30 Process	81
5.15 Cost of Production Estimate for: <i>n</i> -Butanol in China Process: DAVY/Dow <i>n</i> -Butanol LP Oxo Selector 30 Process	82

5.16	Summary of Regional Cost Competitiveness for DAVY/Dow 2-Ethylhexanol LP Oxo Selector 10 Process	83
5.17	Cost of Production Estimate for: 2-Ethylhexanol in Western Europe Process: DAVY/Dow 2-Ethylhexanol LP Oxo Selector 10 Process	85
5.18	Cost of Production Estimate for: 2-Ethylhexanol in China Process: DAVY/Dow 2-Ethylhexanol LP Oxo Selector 10 Process	86
5.19	Summary of Regional Cost Competitiveness for DAVY/Dow 2-Ethylhexanol LP Oxo Selector 30 Process	87
5.20	Cost of Production Estimate for: 2-Ethylhexanol in Western Europe Process: DAVY/Dow 2-Ethylhexanol LP Oxo Selector 30 Process	89
5.21	Cost of Production Estimate for: 2-Ethylhexanol in China Process: DAVY/Dow 2-Ethylhexanol LP Oxo Selector 30 Process	90
5.22	Summary of Regional Cost Competitiveness for DAVY/Dow 2-Propylheptanol LP Oxo Process.....	91
5.23	Cost of Production Estimate for: 2-Propylheptanol in Western Europe Process: DAVY/Dow 2-Propylheptanol LP Oxo Process	93
5.24	Cost of Production Estimate for: 2-Propylheptanol in China Process: DAVY/Dow 2-Propylheptanol LP Oxo Process	94
5.25	Summary of Regional Cost Competitiveness Johnson Matthey Isononanol Process	95
5.26	Cost of Production Estimate for: Isononanol in Western Europe Process: Johnson Matthey	96
5.27	Cost of Production Estimate for: Isononanol in China Process: Johnson Matthey	97
6.1	Global <i>n</i> -Butanol Supply, Demand, and Trade	105
6.2	<i>n</i> -Butanol Capacity in North America	107
6.3	North America <i>n</i> -Butanol Supply, Demand, and Trade	108
6.4	<i>n</i> -Butanol Capacity in Western Europe	110
6.5	Western Europe <i>n</i> -Butanol Supply, Demand, and Trade.....	111
6.6	Asia Pacific <i>n</i> -Butanol Consumption	113
6.7	<i>n</i> -Butanol Capacity in Asia Pacific	115
6.8	Asia Pacific <i>n</i> -Butanol Supply, Demand, and Trade	116
6.9	Global Isobutanol Supply, Demand, and Trade	120
6.10	<i>i</i> -Butanol Capacity in North America	121
6.11	North America Isobutanol Supply, Demand, and Trade	122
6.12	<i>i</i> -Butanol Capacity in Western Europe	123
6.13	Western Europe <i>i</i> -Butanol Supply, Demand, and Trade	124
6.14	Isobutanol Capacity in Asia Pacific	126
6.15	Asia Pacific Isobutanol Supply, Demand, and Trade	127
6.16	Global 2-Ethylhexanol Supply, Demand, and Trade	130
6.17	2-Ethylhexanol Capacity in North America.....	132
6.18	North America 2-Ethylhexanol Supply, Demand, and Trade	133
6.19	2-Ethylhexanol Capacity in Western Europe.....	134

6.20	Western Europe America 2-Ethylhexanol Supply, Demand, and Trade	135
6.21	2-Ethylhexanol Capacity in Asia Pacific	140
6.22	Asia Pacific 2-Ethylhexanol Supply, Demand, and Trade	141
7.1	Risk Assessment Results for Five Phthalates.....	144
7.2	Categorization of Phthalates	145

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

New York: Sonia Ouerani, Client Services Coordinator, NexantThinking™
Phone: +44 207 950 1587 e-mail: souertani@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. 2016. All Rights Reserved.