

C₁₀-Oxo Alcohols

92S1

January 1994

CONTENTS

	Page
I SUMMARY	1
A. INTRODUCTION	1
B. OXO TECHNOLOGY	2
C. COMMERCIAL ANALYSIS	3
1. Applications and Trends	3
2. 2-Propylheptanol	4
3. Oxo Alcohol Feedstocks	6
(a) Oligomers	6
(b) Raffinate-2	7
D. ECONOMIC ANALYSIS	7
II INTRODUCTION	11
A. SELECTION OF PVC PLASTICIZERS	11
B. DEVELOPMENT OF 2-PROPYLHEPTANOL	11
C. THE FUTURE OF FLEXIBLE PVC	14
III OXO TECHNOLOGY	16
A. BACKGROUND	16
1. First Generation - Unmodified Cobalt	17
2. Second Generation - Phosphine-Modified Cobalt	17
3. Third Generation - Phosphine-Modified Rhodium	17
4. Fourth Generation - Bisphosphite-Modified Rhodium	18
B. CLASSIC COBALT	21
1. Isodecanol	21
2. Isononanol	23
C. MODIFIED RHODIUM	24
1. 2-Ethylhexanol	24
(a) Butyraldehyde Production by LP Oxo Synthesis	24
(b) 2-Ethylhexanol Production via Hydrogenation	27

CONTENTS

(Continued)

	Page
2. 2-Propylheptanol	29
(a) Bisphosphite-Modified Catalyst System	30
(b) Valeraldehyde Production by LP Oxo Synthesis	30
(c) 2-Propylheptanol Production via Hydrogenation	34
IV COMMERCIAL ANALYSIS	37
A. C ₈ -C ₁₀ OXO ALCOHOLS	37
1. Applications and Trends	37
2. 2-Propylheptanol and Di-(2-propylheptyl) Phthalate	40
3. Capacity, Supply, and Demand	41
(a) Western Europe	42
(b) United States	44
(c) Japan	46
B. FEEDSTOCKS	47
1. Oligomers	47
(a) Supply	47
(b) Alkylation and Polymerization	50
(c) Octenes from C ₄ Polygas	51
(d) Nonenes from C ₃ Polygas	52
2. Raffinate-2	53
(a) Supply and Demand	53
(b) MTBE	55
V ECONOMIC ANALYSIS	60
A. CASE DESCRIPTIONS	60
1. 2-Ethylhexanol	60
2. Isononanol	60
3. Isodecanol	61
4. 2-Propylheptanol	61

CONTENTS (Continued)

	Page
B. COMPARATIVE ECONOMICS	61
REFERENCES	67
APPENDIX	69
Table A.1	Synthesis Gas from Heavy Fuel Oil
Table A.2	2-Ethylhexanol via Hydroformylation of Propylene
Table A.3	Octenes via Dimerization of Butenes
Table A.4	Isononanol via Hydroformylation of Octenes
Table A.5	Nonenes via Polygas Extraction
Table A.6	Isodecanol via Hydroformylation of Nonenes
Table A.7	2-Propylheptanol via Hydroformylation of Butenes

TABLES

		Page
Table I.B.1	Key Differences Between 2-EH and 2-PH Processes	2
Table I.D.1	C ₈ -C ₁₀ Oxo Alcohols Economic Summary	8
Table I.D.2	C ₈ -C ₁₀ Oxo Alcohols Economics	9
Table III.A.1	Oxo Alcohol Process Development	16
Table III.C.1	Key Differences Between 2-EH and 2-PH Processes	29
Table IV.A.1	West European Oxo Alcohol Consumption for Use in Phthalate Plasticizer Production	40
Table IV.A.2	West European Higher Oxo Alcohol Capacity, 1992	43
Table IV.A.3	West European Higher Oxo Alcohol Supply/Demand Balance and End-Use Breakdown	44
Table IV.A.4	U.S. Higher Oxo Alcohol Capacity, 1992	45
Table IV.A.5	Japanese Higher Oxo Alcohol Capacity, 1992	46
Table IV.B.1	West European Oligomer Capacity, 1992	48
Table IV.B.2	U.S. Oligomer Capacity, 1992	49
Table IV.B.3	Japanese Oligomer Capacity, 1992	49
Table IV.B.4	Typical Disposition of Refinery Butylenes, 1991	51
Table IV.B.5	Typical Disposition of Refinery Propylene, 1991	52
Table IV.B.6	Raffinate-2 Supply/Demand Balance, 1992	55
Table IV.B.7	West European Raffinate-2 Capacity via MTBE	57
Table IV.B.9	U.S. Raffinate-2 Capacity from Raffinate-1 via MTBE	58
Table IV.B.9	Japanese Raffinate-2 Capacity via MTBE	59
Table V.B.1	C ₈ -C ₁₀ Oxo Alcohols Economic Summary	62
Table V.B.2	C ₈ -C ₁₀ Oxo Alcohols Economics	64

FIGURES

		Page
Figure I.C.1	Plasticizer Alcohols' Share of West European Phthalate Plasticizer Market	5
Figure II.B.1	Process Routes to C ₈ -C ₁₀ - Plasticizer Oxo Alcohols	13
Figure III.A.1	Bisphosphite Rhodium Ligand	19
Figure III.A.2	Bisphosphite Structures	20
Figure III.B.1	Oxo Plasticizer-Range Alcohols (Unmodified Cobalt Catalysis)	22
Figure III.C.1	2-Ethylhexanol from Propylene	25
Figure III.C.2	Flow Scheme of LP Oxo Process Using Liquid Recycle	26
Figure III.C.3	Flow Scheme of 2-Ethylhexanol Process	28
Figure III.C.4	Phosphine and Phosphite Ligands	31
Figure III.C.5	2-Propylheptanol Process - Aldehyde Section	32
Figure III.C.6	2-Propylheptanol Process - Aldol and Hydrogenation Section	35
Figure IV.A.1	Plasticizer Alcohols' Share of West European Phthalate Plasticizer Market	39
Figure IV.B.1	Generalized Scheme for Separation of Mixed C ₄ Streams from Steam Cracker Operations	54
Figure V.B.1	C ₈ -C ₁₀ Oxo Alcohols Comparative Economics	63