

Adipic Acid

98/99-3

July 1999

TABLE OF CONTENTS

| | Page |
|--|-------------|
| I EXECUTIVE SUMMARY | 1 |
| A. COMMERCIAL TECHNOLOGY | 1 |
| B. DEVELOPING TECHNOLOGIES | 3 |
| C. ECONOMICS | 4 |
| D. COMMERCIAL ANALYSIS | 10 |
| II CURRENT COMMERCIAL TECHNOLOGY | 14 |
| A. INTRODUCTION | 14 |
| 1. Process Technology | 14 |
| 2. Nitrous Oxide and NOX Generation | 14 |
| B. CHEMISTRY | 16 |
| 1. Air Oxidation of Cyclohexane – Cobalt Catalyst | 16 |
| 2. Air Oxidation of Cyclohexane – Boric Acid Route | 18 |
| 3. Phenol Hydrogenation | 20 |
| 4. Cyclohexanol Via Cyclohexene Hydration | 21 |
| 5. Nitric Acid Oxidation of KA Oil | 22 |
| C. ADIPIC ACID FROM CYCLOHEXANE: BORIC ACID ROUTE | 25 |
| 1. KA Oil Production by the Boric Acid Route | 25 |
| 2. Adipic Acid from KA Oil by Nitric Acid Oxidation | 36 |
| D. ADIPIC ACID FROM CYCLOHEXANE: COBALT CATALYST | 46 |
| 1. KA Oil Production | 46 |
| 2. Nitric Acid Oxidation | 50 |
| E. ADIPIC ACID FROM PHENOL | 51 |
| 1. KA Oil Production | 51 |
| 2. Nitric Acid Oxidation | 54 |
| F. ADIPIC ACID FROM BENZENE VIA CYCLOHEXENE | 55 |
| 1. Cyclohexanol Production | 55 |
| 2. Nitric Acid Oxidation | 61 |
| G. NITROUS OXIDE EMISSIONS REDUCTION SCHEMES | 61 |
| H. LICENSORS | 65 |
| III NEW DEVELOPMENTS | 66 |
| A. SOLUTIA INTEGRATED ADIPIC ACID/PHENOL PROCESS | 66 |
| 1. Solutia Nitrous Oxide Based Phenol Process | 66 |
| 2. Solutia Phenol Process Coupled with Adipic Acid Process | 70 |

TABLE OF CONTENTS (Continued)

| | Page |
|--|----------------|
| B. CYCLOHEXANE OXIDATION DIRECTLY TO ADIPIC ACID BY AIR | 71 |
| C. CYCLOHEXANE OXIDATION BY HYDROGEN PEROXIDE | 73 |
| D. BUTADIENE-BASED ROUTES | 73 |
| 1. Rhone-Poulenc | 74 |
| 2. DuPont/DSM | 74 |
| 3. Union Carbide | 76 |
| E. DIMERIZATION OF METHYL ACRYLATE | 77 |
| IV ECONOMIC ANALYSIS | 79 |
| A. BASIS | 79 |
| 1. Pricing | 79 |
| 2. Investment Basis | 79 |
| 3. Cost of Production Basis | 81 |
| B. COST OF PRODUCTION ANALYSES | 82 |
| 1. KA Oil Via Boric Acid Modified Cyclohexane Oxidation/Adipic Acid | 82 |
| 2. KA Oil Via Cobalt Catalyst/Adipic Acid | 84 |
| 3. KA Oil Via Phenol (Cumene Derived) Hydrogenation/Adipic Acid | 84 |
| 4. Cyclohexanol Via Cyclohexene Hydration/Adipic Acid | 90 |
| 5. KA Oil Via Phenol (Nitrous Oxide) Hydrogenation/Adipic Acid | 90 |
| 6. Speculative Case: BASF Adipic Acid Via Air-Only Cyclohexane Oxidation | 95 |
| C. COMPARATIVE ECONOMICS | 97 |
| D. SENSITIVITIES | 102 |
| V COMMERCIAL STATUS | 105 |
| A. APPLICATIONS | 105 |

**TABLE OF CONTENTS
(Continued)**

| | Page |
|--------------------------|-------------|
| B. UNITED STATES | 106 |
| 1. Demand | 106 |
| 2. Supply | 108 |
| 3. Supply/Demand Balance | 109 |
| C. WESTERN EUROPE | 110 |
| 1. Demand | 110 |
| 2. Supply | 111 |
| 3. Supply/Demand Balance | 112 |
| D. JAPAN | 113 |
| 1. Demand | 113 |
| 2. Supply | 114 |
| 3. Supply/Demand Balance | 114 |
| E. GLOBAL CAPACITY | 115 |
| REFERENCES | 117 |
| APPENDIX A | 119 |
| APPENDIX B | 122 |
| PERP TITLE INDEX | 127 |

TABLES

| | | Page |
|---------------|--|-------|
| Table I.C.1 | U.S. Gulf Coast Summary of KA Oil Economics, 1st Qtr. 1999 | 6 |
| Table I.C.2 | U.S. Gulf Coast Summary of Adipic Acid Process Economics, 1st Quarter 1999 | 8 |
| Table I.D.1 | U.S. Adipic Acid Supply/Demand Balance | 11 |
| Table I.D.2 | West European Adipic Acid Supply/Demand Balance | 11 |
| Table I.D.3 | Japanese Adipic Acid Supply/Demand Balance | 12 |
| Table I.D.4 | Global Adipic Acid Capacity by Producer | 13 |
| Table II.C.1 | Main Design Parameters for KA Oil from Cyclohexane by the Boric Acid Route | 25 |
| Table II.C.2 | Material Balance for KA Oil Production: Boric Acid Route for 488 Million Pound Plant - 8,000 Hours Per Year | 31-35 |
| Table II.C.3 | Main Design Parameters in Adipic Acid Production from KA Oil by Nitric Acid Oxidation | 36 |
| Table II.C.4 | Distribution of Nitric Acid Decomposition Products | 39 |
| Table II.C.5 | Composition of Combined Reactor Gases and Final Vent Gas from Scrubber | 39 |
| Table II.C.6 | Material Balance for Adipic Acid from KA Oil: Nitric Acid Oxidation of KA Oil by Boric Acid Route for 650 Million Pound Plant - 8,000 Hours Per Year | 43-45 |
| Table II.C.7 | Typical Adipic Acid Properties | 46 |
| Table II.D.1 | Effect of KA Oil Manufacturing Method on Material Balances of Nitric Acid Oxidation of KA Oil to Adipic Acid | 51 |
| Table II.F.1 | Effect of Feedstock on Material Balances of Nitric Acid Oxidation of KA Oil/Cyclohexanol to Adipic Acid | 61 |
| Table II.G.1 | Estimated U.S. Emissions of Nitrous Oxide, 1993-1997 | 62 |
| Table III.A.1 | Process Parameters for N ₂ O Oxidation of Benzene to Phenol | 68 |
| Table IV.A.1 | Feedstock and Utility Prices | 80 |
| Table IV.B.1 | Cost Estimate of KA Oil Production via Cyclohexane Oxidation, Boric Acid Route | 83 |

TABLES **(Continued)**

| | Page |
|---|-------------|
| Table IV.B.2 Cost Estimate of Adipic Acid Production via Cyclohexane Oxidation by Air (Boric Acid) and HNO ₃ | 85 |
| Table IV.B.3 Cost Estimate of KA Oil Production via Cyclohexane Oxidation, Cobalt Catalyst | 86 |
| Table IV.B.4 Cost Estimate of Adipic Acid Production via Cyclohexane Oxidation by Air (Cobalt Catalyst) and HNO ₃ | 87 |
| Table IV.B.5 Cost Estimate of KA Oil Production via Gas Phase Phenol (Cumene Derived) Hydrogenation | 88 |
| Table IV.B.6 Cost Estimate of Adipic Acid Production via Phenol (Cumene Derived) Hydrogenation and HNO ₃ Oxidation | 89 |
| Table IV.B.7 Cost Estimate of Cyclohexanol Production via Benzene Hydrogenation, Cyclohexene Hydration | 91 |
| Table IV.B.8 Cost Estimate of Adipic Acid Production via Benzene Partial Hydrogenation, Hydration, and HNO ₃ Oxidation | 92 |
| Table IV.B.9 Cost Estimate of KA Oil Production via Gas Phase Hydrogenation of Phenol from Nitrous Oxide | 93 |
| Table IV.B.10 Cost Estimate of Adipic Acid Production via Hydrogenation of Phenol from Nitrous Oxide, HNO ₃ Oxidation | 94 |
| Table IV.B.11 Cost Estimate of Adipic Acid Production via Single Stage Air Oxidation of Cyclohexane, BASF Patent | 96 |
| Table IV.C.1 Adipic Acid Operating Parameters | 97 |
| Table IV.C.2 U.S. Gulf Coast Summary of KA Oil Process Economics, 1st Qtr. 1999 | 98 |
| Table IV.C.3 U.S. Gulf Coast Summary of Adipic Acid Process Economics, 1st Qtr. 1999 | 100 |
| Table V.B.1 U.S. Adipic Acid Demand | 107 |
| Table V.B.2 U.S. Adipic Acid Capacity, 1998 | 108 |
| Table V.B.3 U.S. Adipic Acid Supply/Demand Balance | 109 |
| Table V.C.1 West European Adipic Acid Demand | 110 |
| Table V.C.2 West European Adipic Acid Capacity, 1998 | 112 |
| Table V.C.3 West European Adipic Acid Supply/Demand Balance | 112 |

TABLES **(Continued)**

| | | Page |
|-------------|--|-------------|
| Table V.D.1 | Japanese Adipic Acid Demand | 113 |
| Table V.D.2 | Japanese Adipic Acid Capacity, 1998 | 114 |
| Table V.D.3 | Japanese Adipic Acid Supply/Demand Balance | 115 |
| Table V.E.1 | Global Adipic Acid Capacity by Producer | 116 |

Appendix Tables

| | | |
|-----------|---|-----|
| Table A.1 | Cost Estimate of Nitric Acid (60%) Production via Mixed Pressure NH ₃ Oxidation | 119 |
| Table A.2 | Cost Estimate of Phenol Production via Benzene/Propylene/ Cumene | 120 |
| Table A.3 | Cost Estimate of Phenol Production via Benzene/Nitrous Oxide (Solutia) | 121 |

FIGURES

| | Page |
|--|-------------|
| Figure I.C.1 Comparison of KA Oil Costs | 7 |
| Figure I.C.2 Comparison of Adipic Acid Costs | 9 |
| Figure II.A.1 Routes to Adipic Acid | 15 |
| Figure II.C.1 KA Oil from Cyclohexane: Boric Acid Route | 27 |
| Figure II.C.2 Adipic Acid from KA Oil via Nitric Acid Oxidation | 37 |
| Figure II.D.1 KA Oil Production by Cobalt Catalyst Route | 48 |
| Figure II.E.1 KA Oil by Phenol Hydrogenation Route | 53 |
| Figure II.F.1 Partial Hydrogenation of Benzene | 57 |
| Figure II.F.2 Extractive Distillation | 58 |
| Figure II.F.3 Cyclohexene Hydration | 59 |
| Figure III.A.1 Simplified Flow Diagram Solutia Process Benzene to Phenol | 69 |
| Figure IV.C.1 Comparison of KA Oil Costs | 99 |
| Figure IV.C.2 Comparison of Adipic Acid Costs | 101 |
| Figure IV.D.1 Feed Price Effect on Adipic Acid Cost | 103 |
| Figure IV.D.2 Capacity Effect on Adipic Acid Cost | 104 |