

BIO ROUTES TO PARA-XYLENE

Table of Contents

A Report by Nexant's CHEMSYSTEMS
Process Evaluation/Research Planning (PERP) Program
PERP 2011S3 - Published March 2012

www.chemsystems.com

Section	Page
1 Executive Summary	1
1.1 INTRODUCTION	1
1.2 RENEWABLE ROUTES TO PARA-XYLENE	2
1.2.1 Dimerization	3
1.2.2 Dehydrocyclization	4
1.3 COMPANIES DOING RESEARCH FOR PRODUCING BIO PARA-XYLENE	4
1.3.1 Anellotech, Inc.	4
1.3.2 Gevo, Inc.	5
1.3.3 Global Bioenergies.....	5
1.3.4 Pacific Northwest National Laboratory (PNNL) and Washington State University (WSU).....	6
1.3.5 UOP.....	7
1.3.6 Virent Energy Systems, Inc.	7
1.4 COMMERCIAL TECHNOLOGY	7
1.5 ECONOMIC ANALYSIS	10
1.6 COMMERCIAL ANALYSIS.....	10
1.6.1 Global.....	10
1.6.2 United States	11
1.6.3 Western Europe.....	12
1.6.4 Asia Pacific	13
1.7 CONCLUSIONS.....	14
2 Bio Technology	16

2.1	INTRODUCTION	16
2.2	RENEWABLE ROUTES TO PARA-XYLENE	17
2.2.1	Dimerization	18
2.2.2	Dehydrocyclization	24
2.3	COMPANIES DOING RESEARCH FOR PRODUCING BIO PARA-XYLENE	28
2.3.1	Anellotech, Inc.	28
2.3.2	Gevo, Inc.	33
2.3.3	Global Bioenergies.....	42
2.3.4	Pacific Northwest National Laboratory (PNNL) and Washington State University (WSU).....	43
2.3.5	UOP.....	43
2.3.6	Virent Energy Systems, Inc.	48
3	Commercial Technology	55
3.1	INTRODUCTION	55
3.2	XYLENES PRODUCTION.....	57
3.2.1	Catalytic Reforming.....	58
3.2.2	Pyrolysis Gasoline	62
3.2.3	Toluene Disproportionation (TDP), Transalkylation, and Dealkylation	64
3.3	XYLENES RECOVERY	75
3.3.1	Introduction.....	75
3.3.2	<i>para</i> -Xylene	78
3.3.3	Isomerization.....	102
3.4	SPECIFICATION	105
4	Economic Analysis	106
4.2	PROCESS ECONOMICS.....	109
4.2.1	Cost of Production	109
4.2.2	Sensitivities.....	121
4.3	CONCLUSIONS.....	127
5	Commercial Analysis	129
5.1	APPLICATIONS OF PARA-XYLENE	129
5.2	GLOBAL	130
5.2.1	Consumption	130
5.2.2	Supply	131

5.2.3	Supply, Demand, and Trade.....	132
5.3	UNITED STATES	134
5.3.1	Consumption	134
5.3.2	Supply	134
5.3.3	Supply, Demand, and Trade.....	136
5.4	WESTERN EUROPE	137
5.4.1	Consumption	137
5.4.2	Supply	138
5.4.3	Supply, Demand, and Trade.....	139
5.5	ASIA PACIFIC	141
5.5.1	Consumption	141
5.5.2	Supply	142
5.5.3	Supply, Demand, and Trade.....	147
6	References	149

Appendix	Page
A List of Acronyms and Abbreviations	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 (2001/2002 - 2011)	D-1

Figure	Page
1.1 How to Make 100 Percent Renewable PET.....	2
1.2 Process Options for Producing <i>para</i> -Xylene from Isobutylene.....	3
1.3 Mixed Xylene Technology	8
1.4 <i>para</i> -Xylene Cost of Production.....	10
1.5 Global <i>para</i> -Xylene Net Trade	11
1.6 United States <i>para</i> -Xylene Supply, Demand, and Trade.....	12
1.7 Western Europe <i>para</i> -Xylene Supply, Demand, and Trade	13
1.8 Asia Pacific <i>para</i> -Xylene Supply, Demand, and Trade.....	14
1.9 Renewable versus Conventional Routes to PX.....	15
2.1 How to Make 100 Percent Renewable PET*	17
2.2 Process Options for Producing <i>para</i> -Xylene from Isobutylene.....	18
2.3 Simplified Block Flow Diagram for Anellotech's Biomass to Aromatics™ Process.....	29
2.4 Proposed Reaction Scheme for Catalytic Fast Pyrolysis	31
2.5 Gevo's Block Flow Diagram for Isobutylene Production	34
2.6 Gevo's Pathway to Isobutanol	35
2.7 Simple Flow Diagram for U.S. Patent Application 2011/0087000	36
2.8 Integrated System to Convert Isobutanol to Renewable <i>para</i> -Xylene	38
2.9 UOP Block Flow Diagram for U.S. Patent 7 439 409.....	46
2.10 Virent's BioForming Process Flow Diagram	50
2.11 Overview of Virent's BioForming® Platform for the Production of Biochemicals and Biofuels	51
2.12 Representative APR Reactant and Product Molecules	52
2.13 GC Compositional Comparison (left) of Virent's BioFormate and a Typical Petroleum Reformate Stream along with a PONA Analysis Comparison (right)	53
3.1 Mixed Xylene Technology	55
3.2 Semi Regenerative Reformer Process Flow Diagram	59
3.3 Continuous Catalytic Reforming Process Flow Diagram.....	60
3.4 Effect of Steam Cracker Feedstock on Aromatics Yield.....	62
3.5 Effect of Severity on BTX Yields for a Full Range Naphtha Feed	63
3.6 Toluene Disproportionation/Transalkylation Typical Flowsheet.....	69
3.7 <i>para</i> -Xylene Production PxMax SM Process Flow Diagram.....	71
3.8 PX-Plus™ Process Flow Diagram.....	74

3.9	Xylenes Recovery Processes.....	76
3.10	Equilibrium Concentrations for C ₈ -Aromatic Compounds.....	78
3.11	<i>para</i> -Xylene Production via UOP Parex™/Isomar Process	81
3.12	Eluxyl® Process Flow Diagram	84
3.13	<i>para</i> -Xylene Production via Crystallization/Isomerization.....	87
3.14	Cascaded Ethylene/Propylene Refrigeration System.....	90
3.15	Single-Effect AAR Cycle	93
3.16	Block Flow Diagram – ExxonMobil PX Crystallization Process.....	101
3.17	Xylenes Isomerization: UOP Isomar Process	103
4.1	BioFormPX Cost of Production Sensitivity to Investment.....	118
4.2	BioFormPX Cost of Production Sensitivity to Hydrogen Price	118
4.3	<i>para</i> -Xylene Cost of Production (USGC, First Quarter 2011)	121
4.4	<i>para</i> -Xylene Cost of Production Sensitivity to Price of Bio Feed.....	122
4.5	Bio <i>para</i> -Xylene Cost of Production Sensitivity to Regional Pricing.....	123
4.6	Bio <i>para</i> -Xylene Cost of Production Sensitivity to Economy of Scale.....	124
4.7	Bio <i>para</i> -Xylene Cost of Production Sensitivity to Investment	125
4.8	Bio <i>para</i> -Xylene Cost of Production plus ROCE.....	126
4.9	Renewable versus Conventional Routes to PX.....	128
5.1	Global <i>para</i> -Xylene End-Use Pattern, 2010	131
5.2	Global <i>para</i> -Xylene Capacity, 2010	132
5.3	Global <i>para</i> -Xylene Net Trade	133
5.4	United States <i>para</i> -Xylene End-Use Pattern, 2010	134
5.5	United States <i>para</i> -Xylene Supply, Demand, and Trade.....	136
5.6	Western Europe <i>para</i> -Xylene End-Use Pattern, 2010.....	137
5.7	Western Europe <i>para</i> -Xylene Supply, Demand, and Trade	140
5.8	Asia Pacific <i>para</i> -Xylene End-Use Pattern, 2010	142
5.9	Asia Pacific <i>para</i> -Xylene Supply, Demand, and Trade.....	148

Table	Page
1.1 Isobutylene to Isooctane Process Comparison Overview	3
1.2 Xylene Demand versus Production.....	9
1.3 Licensors of Aromatics Technology	9
2.1 Isobutylene to Isooctane Process Comparison Overview	18
2.2 InAlk™ Oligomerization Catalyst Comparison.....	19
2.3 Dehydrocyclization Patent Search Results	25
2.4 Material Balance Based on Gevo's U.S. Patent Application 2011/0087000.....	37
2.5 Theoretical Feedstock Consumption for In-situ and Ex-situ Process Platforms	54
3.1 Xylene Demand versus Production.....	56
3.2 Licensors of Aromatics Technology	56
3.3 Typical Composition of Mixed Xylenes.....	57
3.4 Pyrolysis Gasoline Analysis	64
3.5 Reactor Operating Conditions of MSTDP and PxMax SM	72
3.6 C ₈ Aromatics - Physical Properties.....	85
3.7 Typical <i>para</i> -Xylene Specification.....	105
4.1 Feedstock, Byproduct, and Utility Prices	107
4.2 Cost of Production Estimate for: BTX Process: Catalytic Fast Process (CFP)	110
4.3 Cost of Production Estimate for: <i>para</i> -Xylene Process: CFP/Adsorption/Isomerization	111
4.4 Cost of Production Estimate for: Isobutanol Process: Gevo Corn Fermentation	113
4.5 Cost of Production Estimate for: <i>para</i> -Xylene Process: Fermentation followed by Isobutanol Dehydration, Dimerization, Aromatization (with Recycle of Isooctene and Isobutylene) and Recovery	114
4.6 Cost of Production Estimate for: BioFormPX (<i>para</i> -Xylene) Process: BioForming (Using in-situ Hydrogen), Adsorption/Isomerization, TDP, TA.....	116
4.7 Cost of Production Estimate for: BioFormPX (<i>para</i> -Xylene) Process: BioForming (Employing ex-situ Hydrogen), Adsorption/Isomerization, TDP, TA	117
4.8 Cost of Production Estimate for: <i>para</i> -Xylene Process: Naphtha Hydrotreating, Reforming, Adsorption/EB Isomerization, TDP, TA.....	120
5.1 Global <i>para</i> -Xylene Supply, Demand, and Trade	133
5.2 United States <i>para</i> -Xylene Capacity	135
5.3 United States <i>para</i> -Xylene Supply, Demand, and Trade.....	136
5.4 Western Europe <i>para</i> -Xylene Capacity	138

5.5	Western Europe <i>para</i> -Xylene Supply, Demand, and Trade	139
5.6	Asia Pacific <i>para</i> -Xylene Capacity	145
5.7	Asia Pacific <i>para</i> -Xylene Supply, Demand, and Trade.....	147

CHEMSYSTEMS

PERP PROGRAM



www.chemsystems.com

The ChemSystems 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:

London: Dr. Alexander Coker, Manager, PERP Program

Phone: + 44-(20)-7950-1570, e-mail: acoker@nexant.com

New York: Heidi Junker Coleman, Multi-Client Programs Administrator

Phone: + 1-914-609-0381, e-mail: hcoleman@nexant.com

Shanghai: Dr. Y. Larry Song, General Manager, Nexant China

Phone: +86 21 6182 6791, e-mail: ylsong@nexant.com

Nexant, Inc. (www.nexant.com) is a leading management consultancy to the global energy, chemical, and related industries. For over 38 years, ChemSystems 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. 2012. All Rights Reserved.