

**TECHNOLOGY & COSTS****Technoeconomics - Energy & Chemicals (TECH)****TECH 2023-8 Toluene Diisocyanate (TDI)**

## Table of Contents

A Report by **NexantECA, the Energy and Chemical Advisory company**

Published Date: September 2023

[www.nexanteca.com/subscriptions-and-reports](http://www.nexanteca.com/subscriptions-and-reports)**Contents**

1	Executive Summary .....	1
2	Business Overview .....	5
2.1	Introduction.....	5
2.2	Historical Development .....	7
2.3	Business Development.....	8
2.3.1	Toluene Diisocyanate .....	8
2.3.2	Polyurethane Systems .....	9
2.3.3	Polyurethane Processing .....	11
2.4	Barriers to Entry .....	14
2.4.1	Technology .....	14
2.4.2	Market .....	17
2.5	Storage and Handling.....	19
2.6	Physical Properties.....	21
2.6.1	Dinitrotoluene (DNT) .....	21
2.6.2	Toluene Diamine (TDA).....	21
2.6.3	Toluene Diisocyanate (TDI) .....	21
2.7	Regulatory Developments .....	22
3	DNT Process Technology .....	23
3.1	Process Chemistry .....	23
3.2	Mononitration of Toluene.....	25
3.2.1	Mass Transfer .....	26
3.2.2	Chemical Reaction .....	27
3.2.3	Separation of Isomers .....	32
3.2.4	Dinitration of Toluene .....	34
3.3	Selectivity and Conversion.....	34
3.4	Generic Process Technology .....	35
3.4.1	Acid Concentration .....	38
3.5	Chematur Process Technology .....	40
3.6	Josef Meissner Technology.....	42

3.6.1	Company Background.....	42
3.6.2	Process Description .....	42
3.6.3	Reference List .....	45
3.7	Single Acid Nitration .....	45
4	TDI Process Technology .....	48
4.1	Process Chemistry – DNT to TDA .....	48
4.1.1	Catalyst .....	51
4.2	Generic Process Technology - DNT to TDA .....	54
4.3	Process Chemistry - TDA to TDI .....	59
4.4	Generic Process Technology - TDA to TDI.....	61
4.5	Chematur Process Technology .....	67
4.6	BUSS ChemTech Technology .....	69
4.7	HH Chem Tech.....	69
4.8	Covestro Process Technology .....	77
5	Third Party Process Technology .....	83
5.1	Introduction.....	83
5.2	Chloralkali – Chlorine/Caustic Soda.....	84
5.2.1	Overview .....	84
5.2.2	Asahi Kasei Chemical .....	85
5.2.3	BlueStar Chemical.....	86
5.2.4	INEOS Technologies (INOVYN) .....	86
5.2.5	thyssenkrupp Uhde Chlorine Engineers.....	88
5.3	Hydrogen/Carbon Monoxide .....	97
5.3.1	Overview .....	97
5.3.2	Air Liquide .....	97
5.3.3	Linde .....	103
5.3.4	thyssenkrupp Industrial Solutions .....	107
5.4	Nitric Acid .....	115
5.4.1	Overview .....	115
5.4.2	Casale .....	116
5.4.3	DuPont .....	116
5.4.4	Espindesa.....	117
5.4.5	KBR Weatherly.....	117
5.4.6	Stamicarbon .....	118
5.4.7	thyssenkrupp .....	120
6	Process Economics .....	121
6.1	Costing Basis .....	121
6.1.1	Investment Basis .....	121
6.1.2	Pricing Basis.....	121
6.1.3	Cost of Production Basis .....	123
6.2	Cost of Production of Dinitrotoluene .....	124
6.2.1	Assumptions .....	124

6.2.2	Generic DNT Process .....	124
6.2.3	Chematur DNT Process .....	128
6.2.4	Comparison of Process Technologies .....	132
6.3	Cost of Production of Toluene Diisocyanate .....	133
6.3.1	Assumptions .....	133
6.3.2	Generic Process Technology .....	134
6.3.3	Covestro Gas-Phase Process .....	138
6.3.4	Chematur Process Technology .....	142
6.3.5	Comparison of Process Technologies .....	145
6.4	Sensitivity Analysis .....	146
6.4.1	Raw Material Analysis .....	146
6.4.2	Impact of Hydrochloric Acid Economics .....	147
6.4.3	Impact of Third Party Nameplate Capacity .....	148
7	Carbon Intensity .....	149
7.1	Methodology .....	149
7.1.1	Generic Nature of the Analysis .....	149
7.1.2	Carbon Intensity Methodology .....	149
7.2	Results .....	153
8	Commercial Applications .....	155
8.1	Toluene Diisocyanate .....	155
8.1.1	Flexible Foams .....	156
8.1.2	Semi-rigid Foams .....	157
8.1.3	Rigid Foams .....	157
8.1.4	Coatings .....	158
8.1.5	Adhesives .....	159
8.1.6	Elastomers .....	160
9	Market Dynamics .....	162
9.1	Toluene Diisocyanate .....	162
9.1.1	Global Overview .....	162
9.1.2	North America .....	163
9.1.3	Western Europe .....	163
9.1.4	Asia Pacific .....	164
9.1.5	Rest of World .....	165

## Appendices

A	Supporting Cost of Production Estimates .....	167
B	Definitions of Capital Cost Terms Used in Process Economics .....	173
C	Definitions of Operating Costs Terms Used in Process Economics .....	178
D	TECH Program Title Index (2013-2023) .....	181
E	References .....	184

**Figures**

Figure 1	Global TDI Capacity by Marketer .....	1
Figure 2	Global TDI Capacity by Geography .....	2
Figure 3	The Relationship between Raw Material Suppliers and Processors .....	3
Figure 4	Cost of TDI Production by Geography .....	3
Figure 5	Global TDI Carbon Intensity Comparison .....	4
Figure 6	Toluene Diisocyanate Chemical Structure .....	5
Figure 7	The Relationship between Raw Material Suppliers and Processors .....	6
Figure 8	Timeline of Polyurethane Developments .....	7
Figure 9	Routes to Different TDI Product Grades .....	14
Figure 10	Dimerization of TDI .....	19
Figure 11	TDI Dimer Formation at Different Temperatures .....	20
Figure 12	Diisocyanate Saturated Vapor Concentrations .....	20
Figure 13	Nitration of Toluene .....	23
Figure 14	Isomers of DNT .....	23
Figure 15	Mass Transfer Between the Two Liquid Phases .....	25
Figure 16	Mononitration of Toluene .....	28
Figure 17	Ternary Diagram for the Nitric Acid, Sulfuric Acid and Water System .....	30
Figure 18	Oxidation Parasitic Reactions in the Nitration of Toluene .....	31
Figure 19	Phase Diagram for the o/m/p-Nitrotoluene Ternary System (Point D = -40 °C) .....	32
Figure 20	Simplified Flow Diagram of the Separation of the MNT Isomers .....	33
Figure 21	DNT Acid Process Flow Diagram .....	36
Figure 22	DNT Acid Recovery .....	39
Figure 23	DNT Plant .....	40
Figure 24	Chematur DNT process .....	41
Figure 25	Meissner DNT Process Flow Diagram .....	44
Figure 26	DNT Single Acid Process .....	46
Figure 27	Catalytic Hydrogenation of DNT to TDA .....	48
Figure 28	Mass Transfer Limitations in a Heterogeneous Reaction System .....	48
Figure 29	Reaction Scheme for the Catalytic Hydrogenation of 2,4-DNT .....	50
Figure 30	Toluene Diamine Production from DNT .....	55
Figure 31	Fundabac® and Contibac® Filters Configuration .....	56
Figure 32	Dr.M Fundabac® Filter .....	57
Figure 33	Phosgenation reaction of TDA to TDI .....	59
Figure 34	TDI Production via TDA Liquid-Phase Phosgenation: Reaction and Recovery .....	62
Figure 35	TDI Production via TDA Liquid-Phase Phosgenation: Purification .....	64
Figure 36	Typical TDI Residue Processing Facility .....	66
Figure 37	Chematur TDA/TDI .....	68
Figure 38	HH Chem Tech: TDA Phosgenation and Distillation Unit .....	75
Figure 39	HH Chem Tech: T01 Finishing Unit TDI .....	76
Figure 40	TDI Production via TDA Gas-Phase Phosgenation: Reaction and Recovery .....	78
Figure 41	TDI Production via TDA Gas-Phase Phosgenation: Purification .....	80

Figure 42	Typical TDI Residue Processing Facility .....	82
Figure 43	Third-Party Process Technologies .....	83
Figure 44	Membrane Electrolysis Using Oxygen Depolarized Cathodes .....	90
Figure 45	Simplified Flow Diagram of Membrane Electrolyzer with ODC .....	91
Figure 46	Membrane Process – Anodic Reaction .....	92
Figure 47	Diaphragm Flow Diagram .....	93
Figure 48	Diaphragm Cell Electrolysis .....	94
Figure 49	Diaphragm Cell .....	95
Figure 50	Typical Air Liquide HyCO Process Diagram .....	98
Figure 51	Linde's Ammonia Concept LAC.L1 .....	105
Figure 52	Linde Isothermal Shift Reactor .....	106
Figure 53	thyssenkrupp Primary Reformer Design .....	109
Figure 54	tkIS Uhde Hydrogen/Syngas Plant With Pressure Swing Adsorption .....	111
Figure 55	tkIS Direct Process Condensate Reuse System .....	112
Figure 56	Block Flow Diagram of HYCO Plant .....	114
Figure 57	HYCO Plants using thyssenkrupp Technology .....	114
Figure 58	Typical Cost of Production Overview .....	123
Figure 59	DNT Cost of Production by Location .....	132
Figure 60	Comparison of TDI Technology by Region .....	145
Figure 61	Breakdown of Raw Material Costs by Region .....	146
Figure 62	Impact of HCl on TDI Cost of Production .....	147
Figure 63	TDI Cost of Production with Different Third Party Plant Size .....	148
Figure 64	Definition of Scope Emissions .....	149
Figure 65	Process Carbon Balance .....	150
Figure 66	Equation for Utility Emissions .....	151
Figure 67	Equation for Raw Material Emissions .....	152
Figure 68	Global TDI Carbon Intensity Comparison .....	154
Figure 69	Global TDI Consumption by End Use .....	155
Figure 70	Global TDI Capacity by Marketer .....	162
Figure 71	Global TDI Capacity by Region .....	163

## Tables

Table 1	Overview of Processed Polyurethane Products and their Production Process .....	12
Table 2	Technology Barriers to Entry .....	15
Table 3	Current Status of TDI-related Technologies .....	16
Table 4	Availability of Third-party Technologies .....	17
Table 5	Market Barriers to Entry .....	18
Table 6	Distribution of MNT Isomers at Different Temperatures .....	26
Table 7	Heat of Nitration of Toluene .....	28
Table 8	Effect of Temperature in the Mononitration of Toluene .....	28
Table 9	Boiling Point for Mononitrotoluene Isomers .....	32
Table 10	2,4-/2,6-DNT Product Specifications .....	37
Table 11	DNT Plants Using Josef Meissner Technology .....	45
Table 12	JM Sponge Nickel Catalysts .....	53
Table 13	TDA Physical Properties .....	57
Table 14	TDA Commercial Product Specifications .....	58
Table 15	Components Boiling Point at Standard Conditions .....	61
Table 16	Chematur's TDI Product Quality .....	67
Table 17	Comparison of Key Parameters for Different Gas-liquid Reaction Systems .....	70
Table 18	Availability of Third-party Technologies .....	84
Table 19	Chlor-Alkali Plants Using Inovyn Technology .....	88
Table 20	Feedstock and Product Specifications .....	92
Table 21	Diaphragm Cell Feedstock and Product Specifications .....	95
Table 22	HYCO Plants Using Air Liquide Technology .....	103
Table 23	Typical Catalyst Types for Process Units in Syngas Plant .....	108
Table 24	Prices of Raw Materials and Byproducts .....	122
Table 25	Cost of Production Estimate for Dinitrotoluene, USGC Process: Nitration with Mixed Nitric and Sulfuric Acids .....	125
Table 26	Cost of Production Estimate for Dinitrotoluene, Western Europe Process: Nitration with Mixed Nitric and Sulfuric Acids .....	126
Table 27	Cost of Production Estimate for Dinitrotoluene, China Process: Nitration with Mixed Nitric and Sulfuric Acids .....	127
Table 28	Cost of Production Estimate for Dinitrotoluene, USGC Process: Chematur, Nitration with Mixed Nitric and Sulfuric Acids .....	129
Table 29	Cost of Production Estimate for Dinitrotoluene, Western Europe Process: Chematur, Nitration with Mixed Nitric and Sulfuric Acids .....	130
Table 30	Cost of Production Estimate for Dinitrotoluene, China Process: Chematur, Nitration with Mixed Nitric and Sulfuric Acids .....	131
Table 31	Cost of Production Estimate for TDI, USGC Process: Liquid Phase Phosgenation .....	135
Table 32	Cost of Production Estimate for TDI, Western Europe Process: Liquid Phase Phosgenation .....	136
Table 33	Cost of Production Estimate for TDI, China Process: Liquid Phase Phosgenation .....	137
Table 34	Cost of Production Estimate for TDI, USGC Covestro Gas-Phase Process .....	139

Table 35	Cost of Production Estimate for TDI, Western Europe Covestro Gas-Phase Process.....	140
Table 36	Cost of Production Estimate for TDI, China Covestro Gas-Phase Process.....	141
Table 37	Cost of Production Estimate for TDI, USGC Process: Chematur, Catalytic Hydrogenation and Liquid Phase Phosgenation .....	142
Table 38	Cost of Production Estimate for TDI, Western Europe Process: Chematur, Catalytic Hydrogenation and Liquid Phase Phosgenation .....	143
Table 39	Cost of Production Estimate for TDI, China Process: Chematur, Catalytic Hydrogenation and Liquid Phase Phosgenation .....	144
Table 40	Grid Electricity Generation Mix across all Regions .....	151
Table 41	Global TDI Carbon Intensity Comparison.....	154
Table 42	Overview of Preferred Raw Materials for Polyurethanes .....	156
Table 43	Flexible Foam Industries and Applications .....	156
Table 44	Semi-rigid Foam Industries and Applications .....	157
Table 45	Rigid Foam Industries and Applications .....	158
Table 46	Coating Industries and Applications .....	159
Table 47	Adhesive Industries and Applications.....	160
Table 48	Elastomer Industries and Applications .....	161
Table 49	North America TDI Capacity.....	163
Table 50	Western Europe TDI Capacity.....	164
Table 51	Asia Pacific TDI Capacity .....	164
Table 52	Rest of World TDI Capacity .....	165
Table 53	Cost of Production Estimate for Nitric Acid (60 wt%) Process: Conventional Dual Pressure .....	167
Table 54	Cost of Production Estimate for Chlor-Alkali Process: Bipolar Membrane Cell .....	168
Table 55	Cost of Production Estimate for Sulfuric Acid (98 wt% Product, 100 wt% Basis) Process: Contact Process I .....	169
Table 56	Cost of Production Estimate for Synthesis Gas (3:1) Process: Steam Methane Reforming, SMR .....	170
Table 57	Cost of Production Estimate for Hydrogen/Carbon Monoxide Process: Cryogenic Separation from 3:1 Syngas (from SMR) and Purification of H <sub>2</sub> via PSA .....	171
Table 58	Cost of Production Estimate for CO/H <sub>2</sub> Process: Air Liquide, Hydrodesulfurization, Pre-reformer, Reformer, CO <sub>2</sub> Removal (MDEA Unit, BASF license), CH <sub>4</sub> -wash Cold Box including CO Compression, and PSA.....	172



## TECHNOLOGY & COSTS

# Technoeconomics - Energy & Chemicals (TECH)

The NexantECA Subscriptions' Technoeconomics - Energy & Chemicals (TECH) program is recognized globally as the industry standard source for information relevant to the chemical process and refining industries. Technoeconomics - Energy & Chemicals (TECH) reports are available as a subscription program or on a single report basis.

### Contact Details:

#### Americas:

Adam Chan, Managing Consulting  
Phone: + 1-914-609-0326, e-mail: [achan@NexantECA.com](mailto:achan@NexantECA.com)

Erica Hill, Client Services Coordinator, Subscriptions and Reports  
Phone: + 1-914-609-0386, e-mail: [ehill@NexantECA.com](mailto:ehill@NexantECA.com)

#### EMEA:

Anna Ibbotson, Vice President, Sales and Marketing  
Phone: +44-207-950-1528, [aibbotson@NexantECA.com](mailto:aibbotson@NexantECA.com)

#### Asia:

Chommanad Thammanayakatip, Managing Consultant  
Phone: +66-2793-4606, email: [chommanadt@NexantECA.com](mailto:chommanadt@NexantECA.com)

NexantECA Subscriptions and Reports provide clients with comprehensive analytics, forecasts and insights for the chemicals, polymers, energy and cleantech industries. Using a combination of business and technical expertise, with deep and broad understanding of markets, technologies and economics, NexantECA provides solutions that our clients have relied upon for over 50 years.

Copyright © 2000-2023. NexantECA (BVI) Limited. All rights reserved