Abstract
Process Economics Program Report 1F
ALIPHATIC DIISOCYANATES PROCESSES
(February 2002)

Aliphatic and cycloaliphatic diisocyanates (functional groups −N=C=O) are major building blocks in the manufacture of polyurethane products, which are formed by the controlled polyaddition of the diisocyanates with either polyether or polyester polyol coreactants. These diisocyanates are consumed primarily in non-yellowing, high-performance industrial and automotive polyurethane coatings applications.

Industrial scale production of aliphatic and cycloaliphatic diisocyanates has previously been accomplished by the phosgenation of the diamines. However, in recent years, there has been no lack of attempts to prepare these diisocyanates by phosgene-free processes commercially mainly because of phosgene’s corrosivity, high toxicity and high chlorine content. In the mid-1990s, Degussa (previously Creanova or Huls) started-up a 20 million lb/yr IPDI unit in Theodore, Alabama, employing its proprietary phosgene-free urea-based technology; BASF was also believed to have brought on stream a 20 million lb/yr HDI/IPDI swing plant in Germany using a similar patented phosgene-free process.

This report, our sixth on the topic of isocyanates since 1967, presents a comprehensive assessment of the status of the aliphatic and cycloaliphatic diisocyanates industry, primarily HDI and IPDI. It provides a review of current patents and recent business/technology developments, and evaluates major commercial processes. This report also presents two conceptual process designs and economic evaluations for the production of hexamethylene diisocyanate (HDI) and isophorone diisocyanate (IPDI) using non-phosgene urea-based technologies developed by BASF and Degussa. Also presented are updates of the techno-economics in the production of similar scale HDI and IPDI via conventional phosgenation processes. Results of our economic comparison indicate that the phosgene-free urea-based processes are generally more expensive in total fixed capital than their conventional phosgene-based counterparts. Although raw material costs for the non-phosgenation processes are lower, the higher cost of utilities and capital related fixed costs nonetheless result in product values that are 3−7% higher than those obtained via conventional phosgene processes.

In addition, other aliphatic and cycloaliphatic diisocyanates, such as H₁₂MDI (hydrogenated MDI), are also introduced and discussed briefly in the industry status of this report. Overall, this report encompasses the latest technology and process economics, and it provides a basis for insight into technology trends, and possible enhancement in safety and environmental standards with the new phosgene-free routes in the preparation of HDI and IPDI.
CONTENTS

1 INTRODUCTION ........................................................................................................ 1-1

2 SUMMARY ................................................................................................................. 2-1
   GENERAL/MARKET ASPECTS ............................................................................... 2-1
   TECHNOLOGICAL DEVELOPMENTS .................................................................. 2-4
   Non-Phosgenation Processes ............................................................................. 2-4
      Hexamethylene Diisocyanate (HDI) ............................................................... 2-5
      Isophorone Diisocyanate (IPDI) ................................................................ 2-6
   Phosgenation Processes ..................................................................................... 2-7
      Hexamethylene Diisocyanate (HDI) ............................................................... 2-7
      Isophorone Diisocyanate (IPDI) ................................................................ 2-8
   PROCESS ECONOMICS COMPARISON ............................................................... 2-9
      Hexamethylene Diisocyanate (HDI) ............................................................... 2-9
      Isophorone Diisocyanate (IPDI) ................................................................ 2-11

3 INDUSTRY STATUS ................................................................................................. 3-1
   INTRODUCTION ................................................................................................. 3-1
   MAJOR APPLICATIONS ....................................................................................... 3-2
   GLOBAL PRODUCER AND CAPACITY ............................................................. 3-2
   RECENT INDUSTRY DEVELOPMENT ................................................................ 3-5
   PRODUCTION AND CONSUMPTION ................................................................. 3-5
      United States .................................................................................................... 3-5
      Western Europe .................................................................................................. 3-7
      Japan .................................................................................................................. 3-8
   SAFETY AND ENVIRONMENTAL ISSUES ....................................................... 3-8

4 HEXAMETHYLENE DIISOCYANATE (HDI) BY NON-PHOSGENATION PROCESSES ................................................. 4-1
CONTENTS (Continued)

CHEMISTRY.................................................................................................................. 4-1
REVIEW OF PROCESSES ............................................................................................ 4-2
Biscarbamates Formation ............................................................................................. 4-3
Thermal Cleavage ........................................................................................................ 4-5
PROCESS DESCRIPTION .............................................................................................. 4-6
Biscarbamates Formation (Section 100) ..................................................................... 4-7
Thermal Cleavage (Section 100) .................................................................................. 4-7
PROCESS DISCUSSION ................................................................................................. 4-14
Biscarbamates Formation (Section 100) ..................................................................... 4-14
Thermal Cleavage (Section 100) .................................................................................. 4-15
COST ESTIMATES ......................................................................................................... 4-15
Capital Costs ................................................................................................................. 4-15
Production Costs .......................................................................................................... 4-16

5  ISOPHORONE DIISOCYANATE (IPDI) BY NON-PHOSGENATION PROCESSES
................................................................................................................................. 5-1
CHEMISTRY.................................................................................................................. 5-1
IPN Production.............................................................................................................. 5-2
IPDA Production .......................................................................................................... 5-2
IPDI Production............................................................................................................. 5-4
REVIEW OF PROCESSES .......................................................................................... 5-6
IPN Production.............................................................................................................. 5-6
IPDA Production .......................................................................................................... 5-7
IPDI Production............................................................................................................. 5-9
Biscarbamates Formation ......................................................................................... 5-10
Thermal Cleavage ...................................................................................................... 5-11
PROCESS DESCRIPTION ............................................................................................ 5-13
## CONTENTS (Concluded)

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>7-1</td>
</tr>
<tr>
<td>Review of Processes</td>
<td>7-3</td>
</tr>
<tr>
<td>IPDA Phosgenation</td>
<td>7-3</td>
</tr>
<tr>
<td>Product Recovery</td>
<td>7-4</td>
</tr>
<tr>
<td>Process Description</td>
<td>7-5</td>
</tr>
<tr>
<td>IPDI Production (Section 300)</td>
<td>7-5</td>
</tr>
<tr>
<td>Product Purification and Phosgene Recovery (Section 400)</td>
<td>7-5</td>
</tr>
<tr>
<td>Process Discussion</td>
<td>7-19</td>
</tr>
<tr>
<td>IPDI Production (Section 300)</td>
<td>7-19</td>
</tr>
<tr>
<td>Product Purification and Phosgene Recovery (Section 400)</td>
<td>7-19</td>
</tr>
<tr>
<td>Cost Estimates</td>
<td>7-19</td>
</tr>
<tr>
<td>Capital Costs</td>
<td>7-19</td>
</tr>
<tr>
<td>Production Costs</td>
<td>7-20</td>
</tr>
</tbody>
</table>

### Appendix

- **Appendix A: Patent Summary Tables** ............................................. A-1
- **Appendix B: Design and Cost Bases** ............................................. B-1
- **Appendix C: Physical Properties** ............................................... C-1
- **Appendix D: Cited References** .................................................... D-1
- **Appendix E: Process Flow Diagrams** ............................................ E-1
ILLUSTRATIONS

2.1 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation
Effect of Raw Material and Catalyst Costs on Product Value ............................... 2-13

4.1 Hexamethylene Diisocyanate (HDI) Non-Phosgenation ....................................... E-3

5.1 Isophorone Diisocyanate (IPDI) by Non-Phosgenation ........................................ E-5

6.1 Hexamethylene Diisocyanate (HDI) by Phosgenation .......................................... E-9

6.2 Hexamethylene Diisocyanate (HDI) by Phosgenation
Effect of Selectivity and Plant Capacity on Product Value .................................... 6-20

7.1 Isophorone Diisocyanate (IPDI) by Phosgenation .............................................. E-13

7.2 Isophorone Diisocyanate (IPDI) by Phosgenation
Effect of Selectivity and Plant Capacity on Product Value .................................... 7-27
### TABLES

2.1 Average Annual Growth Rates Forecast (2000-2005) ........................................ 2-2
2.2 Major ADI Producers (HDI and IPDI) - Annual Capacity ................................. 2-3
2.3 Process Economics Comparison - HDI ........................................................... 2-10
2.4 Process Economics Comparison - IPDI ......................................................... 2-12
3.1 Major ADI Producers (HDI and IPDI) Annual Capacity - 2001 .................... 3-3
3.2 U.S. Production and Consumption of ADI .................................................... 3-6
3.3 Western European Production and Consumption of ADI ............................. 3-7
3.4 Japan Production and Consumption of ADI - 2000 .................................... 3-8
4.1 Aliphatic Diisocyanates Processes--HDI by Non-Phosgenation Patent Summary ......................................................... A-3
4.2 HDI Non-Phosgenation Design Bases and Assumptions ................................ 4-8
4.3 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation Stream Flows .... 4-9
4.4 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation Major Equipment ................................................................. 4-11
4.5 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation Utilities Summary ................................................................. 4-13
4.6 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation Total Capital Investment ................................................................. 4-17
4.7 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation Production Costs ........................................................................ 4-18
4.8 Hexamethylene Diisocyanate (HDI) by Non-Phosgenation Direct Costs by Section, $ thousands/yr ......................................................... 4-20
5.1 Aliphatic Diisocyanates Processes--IPDI by Non-Phosgenation Patent Summary ......................................................... A-11
5.2 IPDI by Non-Phosgenation Design Bases and Assumptions ................................ 5-16
5.3 Isophorone Diisocyanate (IPDI) by Non-Phosgenation Stream Flows ................................................................. 5-17
5.4 Isophorone Diisocyanate (IPDI) by Non-Phosgenation Major Equipment ................................................................. 5-23
# TABLES (Continued)

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.5</td>
<td>Isophorone Diisocyanate (IPDI) by Non-Phosgenation Utilities Summary</td>
<td>5-27</td>
</tr>
<tr>
<td>5.6</td>
<td>Isophorone Diisocyanate (IPDI) by Non-Phosgenation Total Capital Investment</td>
<td>5-31</td>
</tr>
<tr>
<td>5.7</td>
<td>Isophorone Diisocyanate (IPDI) by Non-Phosgenation Capital Investment by Section</td>
<td>5-32</td>
</tr>
<tr>
<td>5.8</td>
<td>Isophorone Diisocyanate (IPDI) by Non-Phosgenation Production Costs</td>
<td>5-33</td>
</tr>
<tr>
<td>5.9</td>
<td>Isophorone Diisocyanate (IPDI) by Non-Phosgenation Direct Costs by Section, $ thousands/yr</td>
<td>5-35</td>
</tr>
<tr>
<td>6.1</td>
<td>Aliphatic Diisocyanates Processes--HDI by Phosgenation Patent Summary</td>
<td>A-20</td>
</tr>
<tr>
<td>6.2</td>
<td>HDI by Phosgenation Design Bases and Assumptions</td>
<td>6-8</td>
</tr>
<tr>
<td>6.3</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Stream Flows</td>
<td>6-9</td>
</tr>
<tr>
<td>6.4</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Major Equipment</td>
<td>6-10</td>
</tr>
<tr>
<td>6.5</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Utilities Summary</td>
<td>6-12</td>
</tr>
<tr>
<td>6.6</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Total Capital Investment</td>
<td>6-15</td>
</tr>
<tr>
<td>6.7</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Capital Investment by Section</td>
<td>6-16</td>
</tr>
<tr>
<td>6.8</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Production Costs</td>
<td>6-17</td>
</tr>
<tr>
<td>6.9</td>
<td>Hexamethylene Diisocyanate (HDI) by Phosgenation Direct Costs by Section, $ thousands/yr</td>
<td>6-19</td>
</tr>
<tr>
<td>7.1</td>
<td>Aliphatic Diisocyanates Processes--IPDI by Phosgenation Patent Summary</td>
<td>A-23</td>
</tr>
<tr>
<td>7.2</td>
<td>IPDI by Phosgenation Design Bases and Assumptions</td>
<td>7-7</td>
</tr>
<tr>
<td>7.3</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Stream Flows</td>
<td>7-8</td>
</tr>
<tr>
<td>Table</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>-------</td>
<td>-------------</td>
<td>------</td>
</tr>
<tr>
<td>7.4</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Major Equipment</td>
<td>7-14</td>
</tr>
<tr>
<td>7.5</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Utilities Summary</td>
<td>7-18</td>
</tr>
<tr>
<td>7.6</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Total Capital Investment</td>
<td>7-21</td>
</tr>
<tr>
<td>7.7</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Capital Investment by Section</td>
<td>7-22</td>
</tr>
<tr>
<td>7.8</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Production Costs</td>
<td>7-24</td>
</tr>
<tr>
<td>7.9</td>
<td>Isophorone Diisocyanate (IPDI) by Phosgenation Direct Costs by Section, $ thousands/yr</td>
<td>7-26</td>
</tr>
</tbody>
</table>