Abstract
Process Economics Program Report 35D
BUTADIENE AS A CHEMICAL RAW MATERIAL
(September 1998)

The dominant technology for producing butadiene (BD) is the cracking of naphtha to produce ethylene. BD is obtained as a coproduct. As the growth of ethylene production outpaced the growth of BD demand, an oversupply of BD has been created. This situation provides the incentive for developing technologies with BD as the starting material. The objective of this report is to evaluate the economics of BD-based routes and to compare the economics with those of currently commercial technologies. In addition, this report addresses commercial aspects of the butadiene industry such as supply/demand, BD surplus, price projections, pricing history, and BD value in nonchemical applications.

We present process economics for two technologies:
- Cyclodimerization of BD leading to ethylbenzene (DSM-Chiyoda)
- Hydrocyanation of BD leading to caprolactam (BASF).

Furthermore, we present updated economics for technologies evaluated earlier by PEP:
- Cyclodimerization of BD leading to styrene (Dow)
- Carboalkoxylation of BD leading to caprolactam and to adipic acid
- Hydrocyanation of BD leading to hexamethylenediamine.

We also present a comparison of the DSM-Chiyoda and Dow technologies for producing styrene. The Dow technology produces styrene directly and is limited in terms of capacity by the BD available from a world-scale naphtha cracker. The 250 million lb/yr (113,000 t/yr) capacity selected for the Dow technology requires the BD output of two world-scale naphtha crackers. The DSM-Chiyoda technology produces ethylbenzene. In our evaluations, we assumed a scheme whereby ethylbenzene from a 266 million lb/yr (121,000 t/yr) DSM-Chiyoda unit is combined with 798 million lb/yr (362,000 t/yr) of ethylbenzene produced by conventional alkylation of benzene with ethylene. The combined ethylbenzene stream is then dehydrogenated to styrene in a Fina/Badger unit of 1,000 million lb/yr (454,000 t/yr) capacity.
## GLOSSARY

<table>
<thead>
<tr>
<th>Symbol or Term</th>
<th>Definition</th>
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<tbody>
<tr>
<td>ABS</td>
<td>Acrylonitrile-butadiene-styrene</td>
</tr>
<tr>
<td>ACN</td>
<td>6-Aminocapronitrile</td>
</tr>
<tr>
<td>ADA</td>
<td>Adipic acid</td>
</tr>
<tr>
<td>ADN</td>
<td>Adiponitrile</td>
</tr>
<tr>
<td>BD</td>
<td>Butadiene</td>
</tr>
<tr>
<td>BDO</td>
<td>Butanediol</td>
</tr>
<tr>
<td>BLI</td>
<td>Battery limits</td>
</tr>
<tr>
<td>CAPM</td>
<td>Caprolactam</td>
</tr>
<tr>
<td>COD</td>
<td>1,5-Cyclooctadiene</td>
</tr>
<tr>
<td>DMF</td>
<td>Dimethyl formamide</td>
</tr>
<tr>
<td>DMN</td>
<td>Dimethyl naphthalene</td>
</tr>
<tr>
<td>DMT</td>
<td>Dimethyl terephthalate</td>
</tr>
<tr>
<td>EB</td>
<td>Ethylbenzene</td>
</tr>
<tr>
<td>ECH</td>
<td>Ethylcyclohexane</td>
</tr>
<tr>
<td>EPB</td>
<td>3,4-Epoxy-1-butene</td>
</tr>
<tr>
<td>HCN</td>
<td>Hydrocyanic acid</td>
</tr>
<tr>
<td>HMDA</td>
<td>Hexamethylenediamine</td>
</tr>
<tr>
<td>HMI</td>
<td>Hexamethyleneimine</td>
</tr>
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<td>2M2BN</td>
<td>2-Methyl-2-butenenitrile</td>
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<tr>
<td>2M3BN</td>
<td>2-Methyl-3-butenenitrile</td>
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<td>Methyl-2-pentenoate</td>
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<tr>
<td>M4P</td>
<td>Methyl-4-pentenoate</td>
</tr>
<tr>
<td>M5FV</td>
<td>Methyl 5-formylvalerate</td>
</tr>
<tr>
<td>M6AC</td>
<td>Methyl 6-aminocaproate</td>
</tr>
<tr>
<td>MBN</td>
<td>Methyl butenenitrile</td>
</tr>
<tr>
<td>NDA</td>
<td>Naphthalenedicarboxylic acid</td>
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</table>
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<table>
<thead>
<tr>
<th>Symbol or Term</th>
<th>Definition</th>
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<tbody>
<tr>
<td>PBR</td>
<td>Polybutadiene rubber</td>
</tr>
<tr>
<td>PEN</td>
<td>Polyethylene naphthalate</td>
</tr>
<tr>
<td>PN</td>
<td>Pentenenitrile</td>
</tr>
<tr>
<td>Ra-Co</td>
<td>Raney cobalt</td>
</tr>
<tr>
<td>Ra-Ni</td>
<td>Raney nickel</td>
</tr>
<tr>
<td>ROI</td>
<td>Return on investment</td>
</tr>
<tr>
<td>SB</td>
<td>Styrene-butadiene</td>
</tr>
<tr>
<td>SBR</td>
<td>Styrene-butadiene rubber</td>
</tr>
<tr>
<td>TFC</td>
<td>Total fixed capital</td>
</tr>
<tr>
<td>THA</td>
<td>Tetrahydroazepine</td>
</tr>
<tr>
<td>THF</td>
<td>Tetrahydrofuran</td>
</tr>
<tr>
<td>TPB</td>
<td>Triphenylborane</td>
</tr>
<tr>
<td>VCH</td>
<td>Vinylcyclohexene</td>
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