Predicting Chemical Profitability in the Chemical Industry
New Breakthrough Chemical Manufacturing Technologies

George M. Intille
Director, Process Economics Program
SRI Consulting
August 9, 2003
• **PEP** program provides in-depth, independent technical and economic evaluations of both commercial and emerging technologies for the chemical and refining industries.

• **Areas Covered:**
  - Specialty Chemicals
  - Polymers
  - Refining Technologies
  - Life Sciences
  - Environmental Technologies
  - Information Technologies
  - Biotech
A new approach to evaluating technology

Tools:
- Process Simulation
- Equipment Sizing
- Investment Estimation
- Reliable Operating Cost Forecasts
PEP Reviews Almost Every New Petrochemical Development Impacting the Industry

- PET
- Chemicals from Renewable Resources
- Global Petrochemical Outlook
- Sulfur Removal from Petroleum Fuels
- Advances in Oxidation Technology
- Chemicals for Electronic Yearbook 2002
- Chiral Intermediates
- Ethylene Plant Enhancement
- Single Site Catalyst
- Ocean Transportation
- Cogeneration
- Innovative Reactors
- Alpha Olefins
- Membranes
- Aliphatic Diisocyanates
- Super-Absorbant Polymers
- Biocatalysis
- Polypropylene SSC
- Enzymes
- Industrial Coatings
- Non-Metalloccenes
- MeOH Chemicals
- Bio Separations
- Epoxy/Carbonates
- Propylene Industry Outlook
- Alkylation for Motor Fuels
- Octane Improvers
- Propane Based Acrylonitrile
- Refinery Residue Gasification
- Experience Curves
- Biodegradable Polymer Life Cycle Assessment
- Custom Chemical Manufacture
- Strategic Business Units for Nylon
- Polystyrene
- Polypropylene Update
- Natural Gas Liquids
- Acetic Acid
- Fuel Cells for Vehicles and Power
- Propylene Oxide
- DME
- Nano-composites
- Near Zero Sulfur Diesel
- Green Polyurethanes
- Acetal Resins
- Electronic Polymers
- Amino Acids
- Plasticizers
- Fluropolymers
- GTL
Recent Reviews

PEP Review Studies

- Solid Acid Alkylation
- Caprolactam via Gas Phase Beckman Rearrangement
- Basell’s Multizone Circulating Reactor
- ENI Slurry Technology
- Linear Alkylbenzene by Heterogeneous Catalysis
- Methyl Methacrylate
- Maleic anhydride from butane
- Hydroquinone
- Kryoto Update
- Experience Curve Effect on Plant Cost Estimation
- EU 2004 - new country profiles, effect on European chemical markets
- Refrigeration in process plants - CFCs are dead, and HCFCs and HFCs are under pressure
- Zero discharge wastewater strategies
- Online buying and selling of chemicals - a look at the economics
- Breakthrough Technologies
- Self assembling polymers
- Streamlined life cycle assessment of two competing products
- Ethylene vinyl alcohol copolymer
- Glucose
- The (air blown) Starchem Methanol Process
- Carbon Nanotubes for Hydrogen Storage
- Ethanol from Corn Stover
- Acrolein Production (Feed stock for 1,3 propanediol and methionine)
- Glycidyl methacrylate
- Bio computer chips

- Applications of Ionic Liquids
- Elf Atochem Direct route for Hydrogen Peroxide
- Philips Desorb
- Renewable fuel options for gasoline
- Canadian (Alberta) Tar Sands Upgrading
- Homogeneous Solution Polymerization of Fluoromonomers With Supercritical CO2
- Cellulose esters
- Peroxide route to Sulfuric acid
- Catalytic steam cracking for olefins production
- Cell culture processing developments
- Chemical Industry Market Concentration and Scale
- Slurry Phase DME Synthesis Technology.
- Lube Oil dewaxing
- Online, real time economic optimization
- Numerical Methods - overview
- Membrane Applications in natural gas processing
- Barge Mounted GTL Plants
- Membrane desulfurization of refined liquid fuels
- Micro chemical manufacturing
- Computation techniques for estimating physical properties
- Computational fluid dynamics applications in the chemical industry
- Hydotreating Lube Oils
- Methane Hydrate recovery
- Nutritional supplements
- Petroleum coke uses
- Syndiotactic PS & PP
- Valueing intellectual property
Potential “Breakthrough” Technologies Covered in 2003

- Mega Reforming
- Olefin Manufacture via Steam Cracking
- Non-phosgene routes to polycarbonate
- Polystyrene developments
- Propylene Manufacture
- Integration in Petrochemical Complexes
1. Mega Reforming

**Conventional Technology**

- Methane
- Water
- Fuel

Steam Reform → Syngas → Methanol Synthesis

2,000 tons/day

**New Technology**

- Methane
- Water
- Fuel

Steam Reform → ATR → Methanol Synthesis → Methanol

15,000 tons/day
1. Mega Reforming (continued)

**Single-train capacity**
- 2500 tons/day → 5000 tons/day → 15,000 tons/day

**Many new projects**
- Middle East, Australia, Caribbean

**Many active developers**
- Lurgi, Eneos, Halder-Topsoe, Shell, Mitsui, Exxon, Methanex, JGC, many more

**Many technical approaches**
- Compact reforming, Auto-thermal reforming, Combined two-stage reforming, Hot gas reforming, many more
Methanol production costs as low as $50 - $80 per ton

- Reformer → Methanol
- Reformer → Ammonia
- Reformer → DME
- Reformer → Fischer-Tropsch
1. Mega Reforming (continued)

**Impact of Capacity**

**Methanol Capital Investment**
- **Off-Sites**
- **On-Sites**

**Methanol Cost of Production**
- **ROI**
- **Fixed Costs**
- **Variable Cost**

[Graphs showing the impact of capacity on capital investment and cost of production for Methanol.]
1. Mega Reforming (continued)

**Licensor Evaluation**

**Methanol Cost of Production**

- **Dollars per Ton**
  - 0
  - 50
  - 100
  - 150

- **Process**
  - Lurgi
  - Topsoe
  - ICI

- **2,500 tons/day**
- **10,000 tons/day**

**ROI**

**Fixed Costs**

**Variable Cost**
2. Steam Cracking

**Steam Cracking**

\[
\text{Ethane} \rightarrow \text{Ethylene} + \text{Propylene} + \text{Others}
\]

- Very high temperatures
- Very short residence times
2. Steam Cracking (continued)
2. Steam Cracking (continued)

**Economic comparison**

- **Steam Cracking**
  - Ceramic Furnace
  - Conventional

  - Off-Sites
  - On-Sites

  - Variable Costs
  - Fixed Costs
  - ROI

  - Million Dollars
  - Cents per pound

- **Largest volume petrochemical process**
3. Non-phosgene routes to polycarbonate

$$2 \text{ ROH} + \text{ClCCl} \rightarrow \text{ ROCOR} + 2 \text{ HCl}$$

phenol    phosgene    DPC    waste HCl

$$2 \text{ ROH} + \text{CO}_2 \rightarrow \text{ ROCOR} + \text{H}_2\text{O}$$

phenol    carbon dioxide    DPC    water
3. Non-phosgene routes to polycarbonate (continued)

Phosgene

Security and safety concerns
Considered possible WMD

Environmental concerns
Disposal of waste HCl

Corrosion concerns
Aqueous HCl in process

CO and CO₂ alternatives available
3. Non-phosgene routes to polycarbonate (continued)

**Process Options**

- Fixed Bed Carbonylation
- Fluid Bed Carbonylation
- From DMC

**Companies active in catalyst R&D**

- Bayer, Dow, GE, Idemitsu,
- Mitsubishi, MGC, Teijin, Ube,
- Asahi, Daicel
3. Non-phosgene routes to polycarbonate (continued)

Economically competitive processes

- **Diphenyl Carbonate Capital Investment**
  - Fixed Bed
  - Fluid Bed
  - DMC
  - Phosgene

- **Diphenyl Carbonate Cost of Production**
  - Fixed Bed
  - Fluid Bed
  - DMC
  - Phosgene
4. Propylene

**Steam Cracking**

\[ \text{Naphtha} \rightarrow \text{Ethylene} + \text{Propylene} \]

\[ 2 : 1 \]

**MTP/MTO**

\[ \text{Methanol} \rightarrow \text{Ethylene} + \text{Propylene} \]

\[ 1 : 2 \]

**Metathesis**

\[ \text{Butene} + \text{Ethylene} \rightarrow 2 \text{Propylene} \]
4. Propylene (continued)

**Tight propylene market in Asia**

- Increasing ethane based ethylene from Middle East
- Strong demand for polypropylene

**Potential Options**

- Methanol to Propylene
  \[3 \text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{CH} = \text{CH}_2 + 3 \text{H}_2\text{O}\]

- Metathesis
  \[\text{CH}_3\text{CH} = \text{CHCH}_3 + \text{CH}_2 = \text{CH}_2 \rightarrow 2 \text{CH}_3\text{CH} = \text{CH}_2\]

- DCC from refineries

**Active companies**

- Lummus, Lurgi, UOP, Synopec, Stone & Webster, others
4. Propylene (continued)

Alternative to Cracking

**C2 & C3 Olefins**

**Capital Investment**
- MEOH
- Ethane
- Naphtha

**C2 & C3 Olefins**

**Cost of Production**
- ROI
- Fixed Costs
- Variable Cost

**Process**
- Methanol based
- Cracker based

**Costs**
- Methanol based: 25¢/gal
- Cracker based: 40¢/gal
Logistical differences can drive the selection
4. Propylene (continued)

## Integrated Metathesis

<table>
<thead>
<tr>
<th>Products</th>
<th>Naphtha Cracker</th>
<th>Naphtha Cracker plus Methathesis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylene (kmta)</td>
<td>1,000</td>
<td>850</td>
</tr>
<tr>
<td>Propylene (kmta)</td>
<td>500</td>
<td>920</td>
</tr>
<tr>
<td>Butylene (kmta)</td>
<td>300</td>
<td>-</td>
</tr>
<tr>
<td>Olefin Value* ($MM/yr)</td>
<td>855</td>
<td>885</td>
</tr>
<tr>
<td>Investment ($MM)</td>
<td>1,000</td>
<td>1080</td>
</tr>
</tbody>
</table>

Ethylene = $500/ton, Propylene = $500/ton, Butylene = $350/ton
5. Polystyrene developments

PS markets depend on properties and cost
- Packaging (residual monomer)
- Automotive (heat resistance)
- Structural (strength)

No change in Ziegler-Natta process since 1970s
- Free radical catalyzed polymerization

Anionic processes - explosively uncontrolable
- Rapid rate – highly exothermic

Active developers
- Dow, Mitsubishi
5. Polystyrene developments (continued)

Competitive investment and operating costs

Polystyrene Capital Investment

<table>
<thead>
<tr>
<th>Process</th>
<th>Off-Sites (Million Dollars)</th>
<th>On-Sites (Million Dollars)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPP</td>
<td>40</td>
<td>20</td>
</tr>
<tr>
<td>HIPS</td>
<td>60</td>
<td>40</td>
</tr>
</tbody>
</table>

Polystyrene Cost of Production

<table>
<thead>
<tr>
<th>Process</th>
<th>ROI (Dollars per Ton)</th>
<th>Fixed Costs (Dollars per Ton)</th>
<th>Variable Cost (Dollars per Ton)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPP</td>
<td>1,200</td>
<td>800</td>
<td>400</td>
</tr>
<tr>
<td>HIPS</td>
<td>1,600</td>
<td>1,200</td>
<td>400</td>
</tr>
</tbody>
</table>

## Lower cost

## Lower residual monomer

## Higher strength

<table>
<thead>
<tr>
<th>Trait</th>
<th>Conventional Free Radical</th>
<th>New Anionic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Capacity</td>
<td>68,000 tons/yr</td>
<td>Same</td>
</tr>
<tr>
<td>Capital investment cost</td>
<td>$30 million</td>
<td>$28 million</td>
</tr>
<tr>
<td>Production cost</td>
<td>$992/ton</td>
<td>$860/ton</td>
</tr>
<tr>
<td>Residual monomer</td>
<td>200 ppm</td>
<td>10 ppm</td>
</tr>
</tbody>
</table>
6. Integration in petrochemical complexes

**Integrated olefin manufacturing sites**

- 3+ Million tons per year
- Extremely complex multi-product production
- $10+ Billion dollar investments

**Numerical methods – Simpler & Faster**

- e.g. Refinery LPs are commonly run once per shift or more

**Many active developers**

- Aspen, SymSy, Honeywell, Invensys, SRIC, many more

**Many opportunities for optimization**

- Savings can exceed 5% of total revenue
6. Integration in major petrochemical complexes (continued)

Integrated multi-product sites – even more so

- Power
- Utilities
- Off sites
- MeOH
- LSR
- Naphtha
- Condensate
- NGLs
- Pipelines
- Ethylene Plant 1
- Ethylene Plant 2
- Ethylene Plant 3
- MTP
- Metathesis
- Polymers
- Aromatics
- Chemicals
- Ethylene
- Propylene
- Terminals
- Docks
- Products
## Traits common to refineries and petrochemical complexes

<table>
<thead>
<tr>
<th>Trait</th>
<th>PC Complex</th>
<th>Refinery</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiple feeds</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Multiple products</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Multiple unit operations</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Multiple intermediate streams</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Complex storage and shipping</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Online integrated optimization</td>
<td>No</td>
<td>Often</td>
</tr>
<tr>
<td>Daily optimization</td>
<td>Rarely</td>
<td>Always</td>
</tr>
<tr>
<td>Potential benefit of optimization</td>
<td><strong>5-10%</strong></td>
<td><strong>5-10%</strong></td>
</tr>
</tbody>
</table>
Evaluation of commercial potential is potent research stimulus