







CHEMRAWN XVI CONFERENCE

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

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- 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



### Studies 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-Metallocenes **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



### **PEP Review Studies**

- Solid Acid Alkylation
- Caprolactam via Gas Phase Beckman Rearrangement
- **Basell's Multizone Circulating Reactor**
- **ENI Slurry Technology**
- Linear Alkylbenzene by Hetergeneous 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

# Reviews



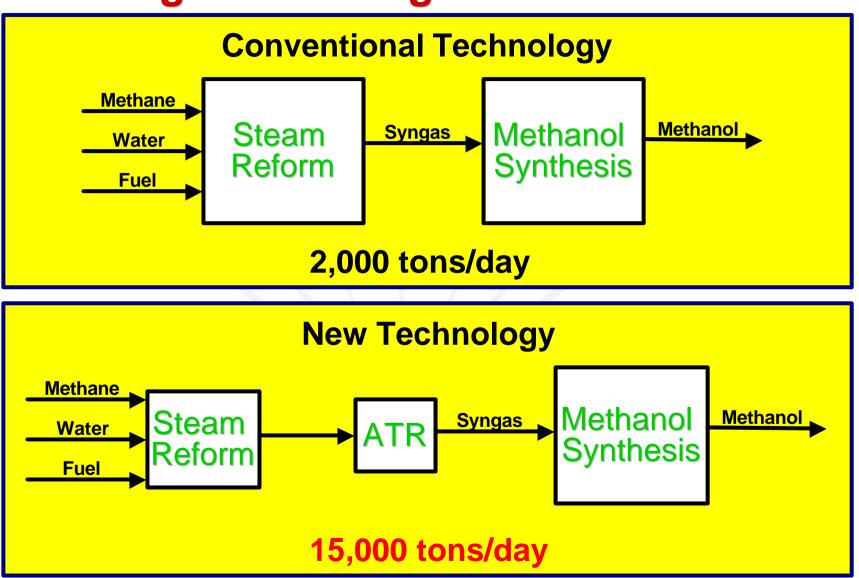


# Potential "Breakthrough" Technologies Covered in 2003

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



# . Mega Reforming



Mega

Reforming





Single-train capacity 2500 tons/day  $\rightarrow$  5000 tons/day  $\rightarrow$  15,000 tons/day

Many new projects

Middle East, Australia, Carribean

### Many active developers

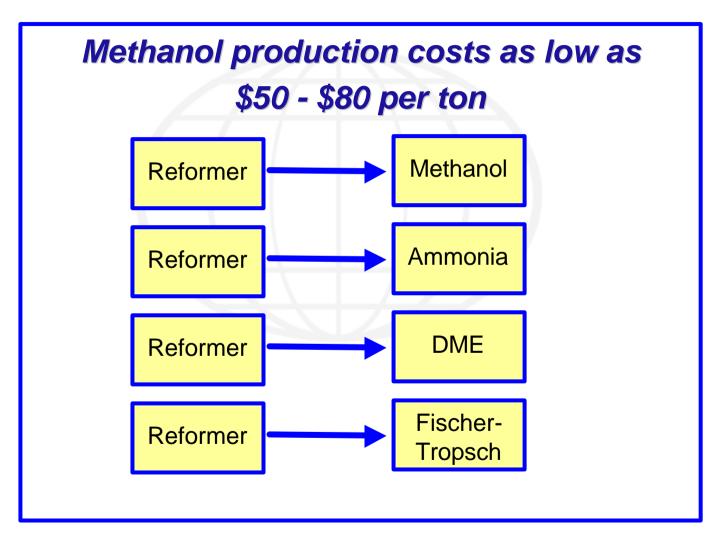
Lurgi, Eneos, Halder-Topsoe,, Shell, Mitsui, Exxon, Methanex, JGC, many more

## Many technical approaches

Compact reforming, Auto-thermal reforming, Combined twostage reforming, Hot gas reforming, many more

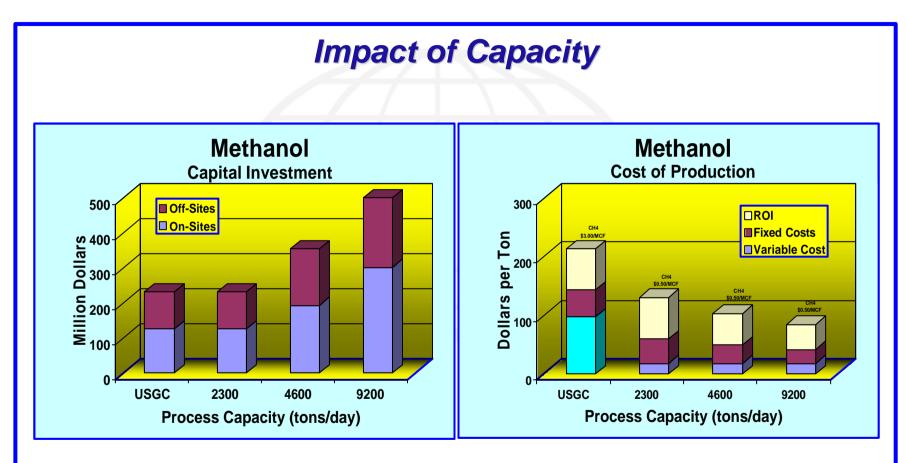






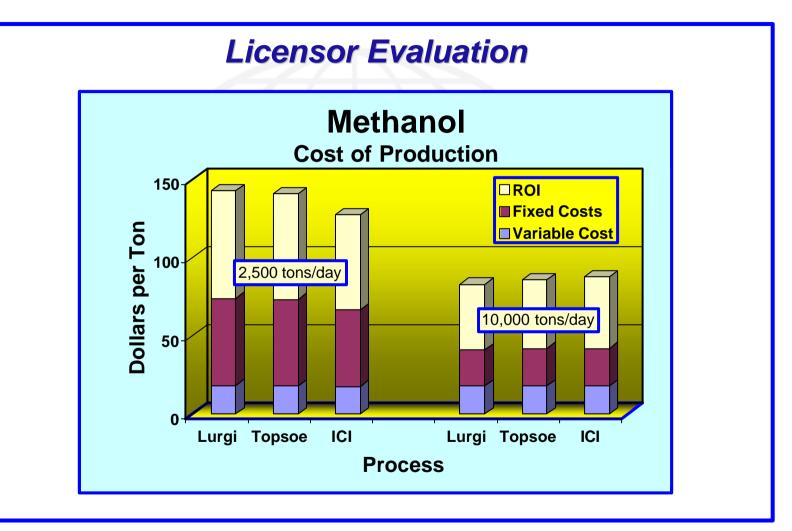














**Steam Crackin** 

# 2. Steam Cracking

# Steam Cracking

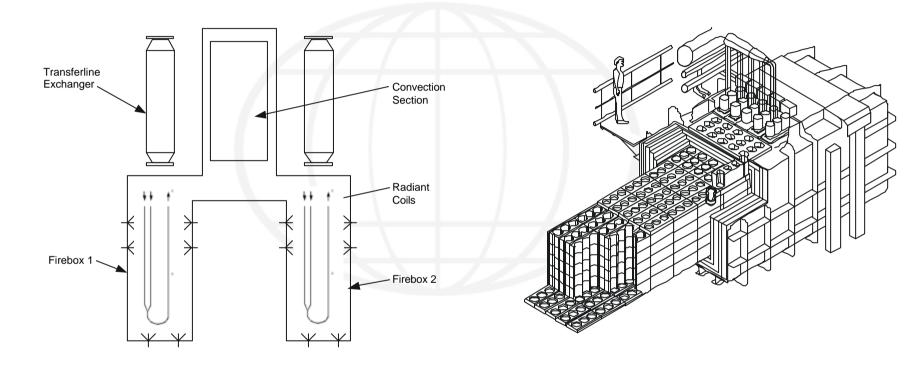
Ethane  $\rightarrow$  Ethylene + Propylene + Others

Very high temperaturesVery short residence times



### **Steam Crackin**

#### 2. Steam Cracking(continued)





### **Steam Cracking**

### 2. Steam Cracking(continued)

Conventional

**Ceramic Furnace** 

#### **Economic comparison Steam Cracking Steam Cracking** 500 30 Cents per pound 400 Million Dollars 20-**■Off-Sites** 300 □Variable Costs □On-Sites Fixed Costs 200 10 100 0 0

Largest volume petrochemical process

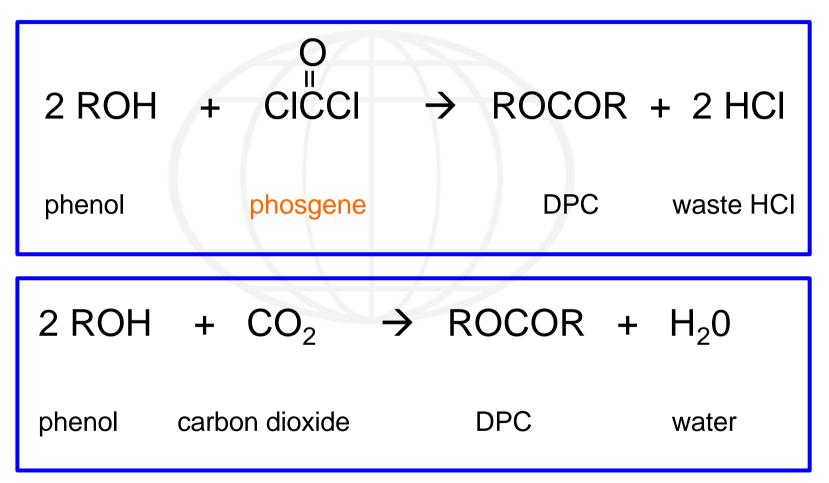
**Ceramic Furnace** 

Conventional



Polycarbonates

# 3. Non-phosgene routes to polycarbonate







### 3. Non-phosgene routes to polycarbonate (continued)

# Phosgene

Security and safety concerns

Considered possible WMD

**Environmental concerns** 

Disposal of waste HCI

**Corrosion concerns** 

Aqueous HCI in process

**CO and CO<sub>2</sub> alternatives available** 



Polycarbonates

3. Non-phosgene routes to polycarbonate (continued)

**Process Options** 

Fixed Bed Carbonylation Fluid Bed Carbonylation From DMC

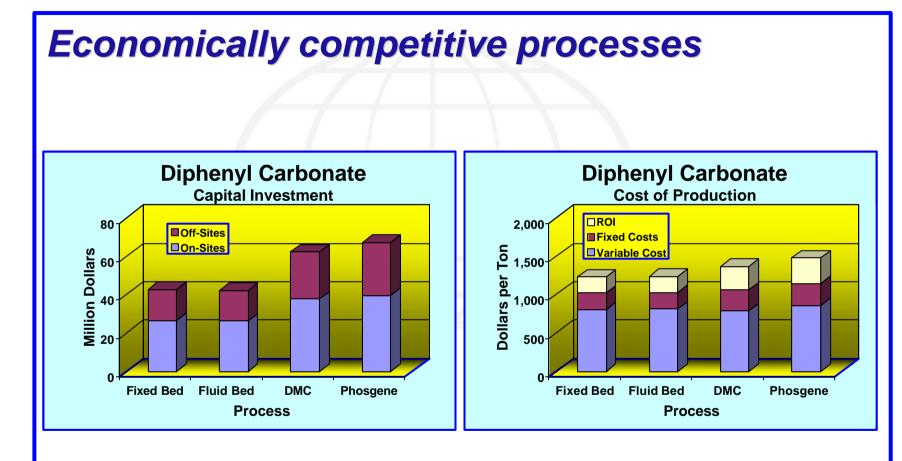
**Companies active in catalyst R&D** 

Bayer, Dow, GE, Idemitsu, Mitsubishi, MGC, Teijin, Ube, Asahi, Daicel



Polycarbonates

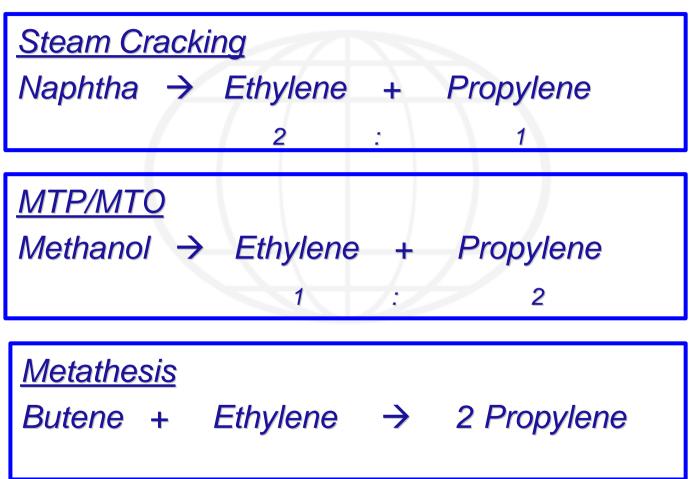
### 3. Non-phosgene routes to polycarbonate (continued)





Propylene

# 4. 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  $3 CH_3OH \rightarrow CH_3CH=CH_2 + 3 H_2O$ Metathesis  $CH_3CH=CHCH_3 + CH_2 = CH_2 \rightarrow 2 CH_3CH=CH_2$ DCC from refineries Active companies Lummus, Lurgi, UOP, Synopec, Stone & Webster, others





#### 4. Propylene (continued)

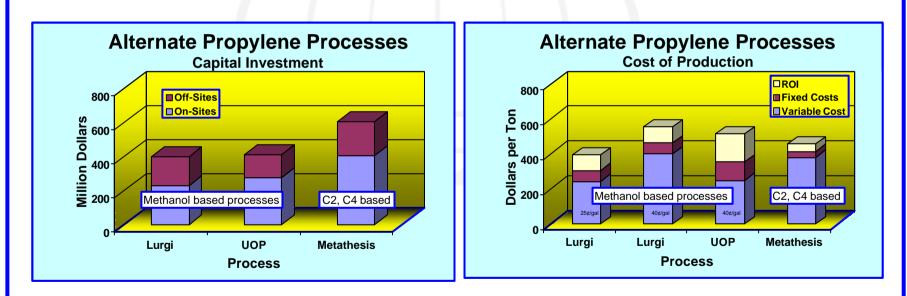
#### Alternative to Cracking C2 & C3 Olefins C2 & C3 Olefins **Cost of Production Capital Investment** 800 800 ■Off-Sites Fixed Costs Willion Dollars □On-Sites **□Variable Cost Million Dollars** 600<sup>-</sup> 400-Cracker based Methanol based 200 Methanol based Cracker based 25¢/gal 40¢/ga 0-0 MEOH Naphtha MEOH MEOH Ethane Naphtha Ethane **Process Process**



### Propylene

### 4. Propylene (continued)

### **Methanol vs Metathesis**



Logistical differences can drive the selection





### 4. Propylene (continued)

## **Integrated Metathesis**

Products	Naphtha Cracker	Naphtha Cracker plus Methathesis
Ethylene (kmta)	1,000	850
Propylene (kmta)	500	920
Butylene (kmta)	300	-
Olefin Value* (\$MM/yr)	855	885
Investment (\$MM)	1,000	1080

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

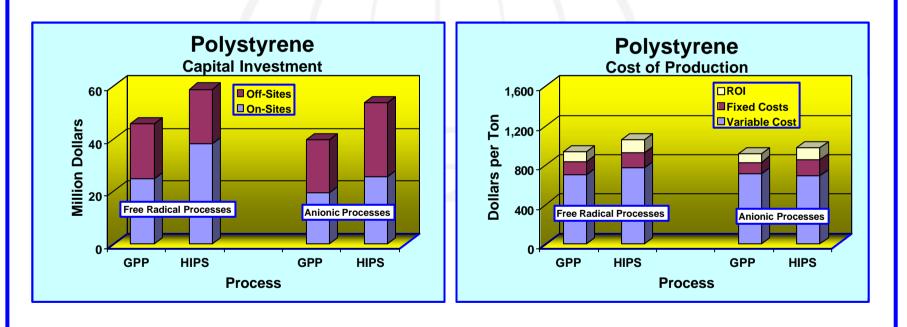
Dow, Mitsubishi



Polystyrene

### 5. Polystyrene developments (continued)

# **Competitive investment and operating costs**





### 5. Polystyrene developments (continued)

### Lower cost

- Lower residual monomer
- **Higher strength**

Trait	Conventional	New
	Free Radical	Anionic
Capacity	68,000 tons/yr	Same
Capital investment cost	\$30 million	\$28 million
Production cost	\$992/ton	\$860/ton
Residual monomer	<b>200 ppm</b>	10 ppm



Integration

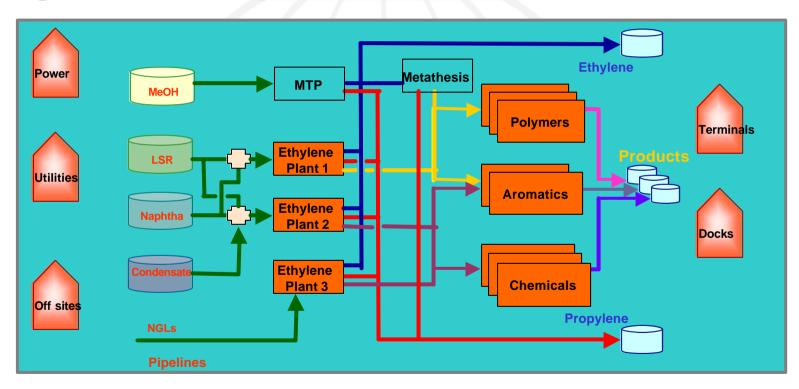
# 6. Integration in petrochemical complexes Integrated olefin manufacturing sites 3+ Million tons per year Extremely complex multi-product production \$10+ Billion dollar investments Numerical methods – Simpler & Faster e.g. Refinery LPs are commonly run once per shift or more Many active developers Aspen, SymSy, Honeywell, Invensys, SRIC, many more Many opportunities for optimization Savings can exceed 5% of total revenue



Integration

### 6. Integration in major petrochemical complexes (continued)

### Integrated multi-product sites – even more so





Integration

6. Integration in major petrochemical complexes (continued)

Traits common to refineries and petrochemical complexes

Trait	PC Complex	Refinery
Multiple feeds	Yes	Yes
Multiple products	Yes	Yes
Multiple unit operations	Yes	Yes
Multiple intermediate streams	Yes	Yes
Complex storage and shipping	Yes	Yes
Online integrated optimization	Νο	Often
Daily optimization	Rarely	Always
Potential benefit of optimization	5-10%	5-10%

Evaluation of commercial potential is potent research stimulus

