Sources of Information on Manufacturing Processes

- The information that is published on commercial processes is restricted.

- Technical literature and textbooks give only a superficial account of the chemistry and unit operations used. However it is useful in the early stages of a project, when searching for possible process routes.

- It is important to make a thorough search of the literature to obtain the latest data.
Sources of Information on Manufacturing Processes

- **Indexes**
  - *Chemical Abstracts, since 1907* (> 15,000 sci. & eng. journals, patents from 26 countries)
  - *Engineering Index*
  - *Applied Science and Technology Index*
  - *Science Citation Index*

- **Handbooks**
  - *Perry's Chemical Engineers' Handbook*
  - *Handbook of Chemistry and Physics*
  - *Chemical Processing Handbook*
  - *Unit Operations Handbook*
  - *Data for Process Design and Engineering Practice*
  - *Riegel's Handbook of Industrial Chemistry*
  - *JANAF Thermochemical Tables*

- **Books:**
  - *SRI (Stanford Research Institute) Design Reports*
  - *Encyclopedia of Chemical Technology* edited by Kirk & Othmer
  - *Ullmann's Encyclopedia of Industrial Technology*, Ullmann
  - *Encyclopedia of Chemical Processing and Design*
  - *McGraw-Hill Encyclopedia of Science and Technology*
  - *Van Nostrand's Scientific Encyclopedia*
  - *Encyclopedia of Materials Science and Engineering*
  - *Handbook of Reactive Chemical Hazards*
  - *Toxic Chemical Release Inventory (TCRI)*
  - *Handbook of Toxic and Hazardous chemicals*

Books quickly become outdated. Journals are more up-to-date.
Sources of Information on Manufacturing Processes

- **Patents**
  - Patents can be a useful source of information, but some care is needed in extracting information from them.
  - When using data from patents, it is important to carefully read the section that describes the experimental procedure to be sure that the experiments were run under appropriate conditions.
  - “the reaction is carried out at a temperature in the range 50 to 500 ℃, more preferably in the range 100 to 300 ℃, and most preferably in the range 200 to 250 ℃.”

FLOWSHEETING

- The flowsheet, the key document in process design is a **diagrammatic model** of the process.
- During plant startup and subsequent operation, the flowsheet forms a basis for comparison of operating performance with design.
- Piping and Instrument diagrams (P & I or PIDs), or engineering flowsheet or mechanical flowsheet shows the engineering details of the process.
Block Diagrams

- Block diagram is the simplest form of presentation. Each block can represent a single piece of equipment or a complete stage in the process.

- They are useful for showing simple processes. With complex processes, their use is limited to showing the overall process, broken down into its principal stages.

- Block diagrams are useful for representing a process in a simplified form in reports, textbooks, and presentations, but have only limited use as engineering documents.

- Block diagrams are often drawn using simple graphics programs such as Visio™ or Microsoft PowerPoint™.
Pictorial Representation

- There are several international standards for PFD symbols, but most companies use their own standard symbols, as the cost of converting all of their existing drawings would be excessive.

- ISO 10628 is the international standard for PFD drawing symbols. Very few North American companies apply this standard.


---

BS 1553

<table>
<thead>
<tr>
<th>Heat exchanger (basic symbols)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternative:</td>
<td></td>
</tr>
<tr>
<td>Shell and tube: fixed tube sheet</td>
<td></td>
</tr>
<tr>
<td>Shell and tube: U tube or floating head</td>
<td></td>
</tr>
<tr>
<td>Shell and tube: kettle reboiler</td>
<td></td>
</tr>
<tr>
<td>Air-blown cooler</td>
<td></td>
</tr>
</tbody>
</table>
Nitric acid Production flowsheet

Precision of data

- Imprecise small flows are best shown as “TRACE.” If the composition of a trace component is specified as a process constraint, as, say, for an effluent stream or product quality specification, it can be shown in parts per million (ppm).

- Trace quantities can be important. Only a trace of an impurity is needed to poison a catalyst, and trace quantities can determine the selection of the materials of construction.
THE PRELIMINARY DESIGN

Example

- The research division of a petroleum company has suggested that a very promising area in the petrochemical field would be in the development and manufacture of biodegradable synthetic detergents using some of the hydrocarbon intermediates presently available in the refinery.

- A survey by the market division has indicated that the company could hope to attain 2.5 percent of the detergent market if a plant with an annual production of 15 million pounds were to be built.

Literature Survey

- A survey of the literature reveals that the majority of the detergents are alkylbenzene sulfonates (ABS). Theoretically, there are over 80,000 isomeric alkylbenzenes in the range of C_{10} to C_{15} for the alkyl side chain.

- Costs, however, generally favor the use of dodecene (propylene tetramer) as the starting material for ABS.

- There are many different schemes in the manufacture of ABS. Most of the schemes are variations of the one shown in Fig. 2-3.
Production of sodium dodecylbenzene sulfonate

Alkylation:

\[
C_6H_6 \cdot C_{12}H_{24} \xrightarrow{\text{AlCl}_3} C_6H_5 \cdot C_{12}H_{25}
\]

Sulfonation:

\[
C_6H_5 \cdot C_{12}H_{25} + H_2SO_4 \rightarrow C_{12}H_{25} \cdot C_6H_4 \cdot SO_3H + H_2O
\]

Neutralization:

\[
C_{12}H_{25} \cdot C_6H_4 \cdot SO_3H + NaOH \rightarrow C_{12}H_{25} \cdot C_6H_4 \cdot SO_3Na + H_2O
\]

This process involves reaction of dodecene with benzene in the presence of aluminum chloride catalyst;

\textbf{fractionation} of the resulting crude mixture to recover the desired boiling range of dodecylbenzene;

\textbf{sulfonation} of the dodecylbenzene;

subsequent \textbf{neutralization} of the sulfonic acid with caustic soda;

\textbf{blending} the resulting slurry with chemical “builders”, and drying.
Production of sodium dodecylbenzene sulfonate

- Dodecene is charged into a reaction vessel containing benzene and aluminum chloride.
- The reaction mixture is agitated and cooled to maintain the reaction temperature of about 115°F maximum.
- An excess of benzene is used to suppress the formation of by-products. Aluminum chloride requirement is 5 to 10 wt% of dodecene.

After removal of aluminum chloride sludge, the reaction mixture is fractionated to recover excess benzene (which is recycled to the reaction vessel), a light alkylaryl hydrocarbon, dodecylbenzene, and a heavy alkylaryl hydrocarbon.
Production of sodium dodecylbenzene sulfonate

- Sulfonation of the dodecylbenzene may be carried out continuously or batch-wise under a variety of operating conditions using sulfuric acid (100 percent), oleum (usually 20 percent SO₃), or anhydrous sulfur trioxide.

- The optimum sulfonation temperature is usually in the range of 100 to 140°F depending on the strength of acid employed, mechanical design of the equipment, etc.

- Removal of the spent sulfuric acid from the sulfonic acid is facilitated by adding water to reduce the sulfuric acid strength to about 78 percent.

- This dilution prior to neutralization results in a final neutralized slurry having approximately 85 percent active agent based on the solids.

- The inert material in the final product is essentially Na₂SO₄.
Production of sodium dodecylbenzene sulfonate

- The sulfonic acid is neutralized with 20 to 50 percent caustic soda solution to a pH of 8 at a temperature of about 125°F.

- Chemical "builders" such as trisodium phosphate, tetrasodium pyrophosphate, sodium silicate, sodium chloride, sodium sulfate, carboxymethyl cellulose, etc., are added to enhance the detersive, wetting, or other desired properties in the finished product. A flaked, dried product is obtained by drum drying or a bead product is obtained by spray drying.

THE PRELIMINARY DESIGN

Example

- The basic reactions which occur in the process are the following.
  
  **Alkylation:**
  \[ \text{C}_6\text{H}_6 + \text{C}_{12}\text{H}_{25} \xrightarrow{\text{AlCl}_3} \text{C}_6\text{H}_5 \cdot \text{C}_{12}\text{H}_{25} \]
  
  **Sulfonation:**
  \[ \text{C}_6\text{H}_5 \cdot \text{C}_{12}\text{H}_{25} + \text{H}_2\text{SO}_4 \longrightarrow \text{C}_{12}\text{H}_{25} \cdot \text{C}_6\text{H}_4 \cdot \text{SO}_3\text{H} + \text{H}_2\text{O} \]
  
  **Neutralization:**
  \[ \text{C}_{12}\text{H}_{25} \cdot \text{C}_6\text{H}_4 \cdot \text{SO}_3\text{H} + \text{NaOH} \longrightarrow \text{C}_{12}\text{H}_{25} \cdot \text{C}_6\text{H}_4 \cdot \text{SO}_3\text{Na} + \text{H}_2\text{O} \]

- A literature search indicates that yields of 85 to 95 percent have been obtained in the alkylation step, while yields for the sulfonation process are substantially 100 percent, and yields for the neutralization step are always 95 percent or greater.
THE PRELIMINARY DESIGN
Example

- All three steps are exothermic and require some form of jacketed cooling around the stirred reactor to maintain isothermal reaction temperatures.
- Laboratory data for the sulfonation of dodecylbenzene, described in the literature, provide additional information useful for a rapid material balance.

1. Sulfonation is essentially complete if the ratio of 20 percent oleum to dodecylbenzene is maintained at 1.25.
2. Spent sulfuric acid removal is optimized with the addition of 0.244 lb of water to the settler for each 1.25 lb of 20 percent oleum added in the sulfonation step.
3. A 25 percent excess of 20 percent NaOH is suggested for the neutralization step.

Material and Energy Balance

- The process selected for the manufacture of the nonbiodegradable detergent is essentially continuous even though the alkylation, sulfonation, and neutralization steps are semicontinuous steps.
- Provisions for possible shutdowns for repairs and maintenance are incorporated into the design of the process by specifying plant operation for 300 calendar days per year.
- Assuming 90 percent yield in the alkylation and a sodium dodecylbenzene sulfonate product to be 85 percent active with 15 percent sodium sulfate as inert, the overall material balance is as follows:

\[
\text{Product (85\% active)} = \frac{(15 \times 10^6)(0.85)}{(300)(348.5)} = 122 \text{ lb mol/day}
\]
Material and Energy Balance

\[ C_6H_6 \text{ feed} = (122) \left( \frac{1}{0.95} \right) \left( \frac{1}{0.90} \right) = 142.7 \text{ lb mol/day} \]
\[ = (142.7 \times 78.1) = 11,145 \text{ lb/day} \]
\[ C_{12}H_{24} \text{ feed} = 142.7 \text{ lb mol/day} \]
\[ = (142.7 \times 168.3) = 24,016 \text{ lb/day} \]

20% oleum in = \( (1.25)(11,145 + 24,016) = 43,951 \text{ lb/day} \)
Dilution \( H_2O \) in = \( (0.244 / 1.25)(43,951) = 8579 \text{ lb/day} \)
20% \( NaOH \) in = \( (1.25)(43,951) = 55,085 \text{ lb/day} \)
\( AlCl_3 \) catalyst in = \( (0.05)(11,145 + 24,016) = 1758 \text{ lb/day} \)
Equipment Design and Selection

- Equipment design for this preliminary process evaluation involves determining the **size of the equipment** in terms of the volume, flow per unit time, or surface area. Some of the calculations associated with the alkylation unit are presented in the following.

- **ALKYLATION UNIT EQUIPMENT**

- **DESIGN AND SELECTION**

- Assume a 4-h cycle and operation of the alkylation unit at constant temperature and pressure of **115°F** and **1 atm**, respectively. The volume of reactants per day (with a 10% safety factor) is

  \[
  V = (12,259) + (26,418) + (1758)(7.48)
  \]

  \[
  = (8.34)(0.88) + (8.34)(0.7533) + (2.44)(62.4)
  \]

  \[
  = 1670 + 4160 + 86 = 5916 \text{ gal/day}
  \]

  \[
  = 5916 \div 6 = 986 \text{ gal/cycle}
  \]

- If the reactor is 75% full on each cycle, the volume of reactor needed is

  \[
  V_R = \frac{986}{0.75} = 1315 \text{ gal}
  \]

- Select a 1300-gal, glass-lined, stirred reactor.

- **HEAT OF REACTION CALCULATION**

  \[
  \Delta H_r = \Delta H_{f(C_6H_5)} + \Delta H_{f(C_{12}H_{25})} - \Delta H_{f(C_6H_5)} - \Delta H_{f(C_{12}H_{25})}
  \]
Equipment Design and Selection

The heats of formation $\Delta H_f$ of dodecylbenzene and dodecene are evaluated using standard thermochemistry techniques outlined in most chemical engineering thermodynamic texts. The heat formation of benzene is available in the literature.

\[
\begin{align*}
\Delta H_{f\text{C}_{12}H_{25}O} &= -54,348 \text{ cal/g mol} \\
\Delta H_{f\text{C}_{10}H_{20}O} &= -51,239 \text{ cal/g mol} \\
\Delta H_{f\text{C}_{8}H_{18}O} &= 11,717 \text{ cal/g mol} \\
\Delta H_r &= -54,348 + 11,717 + 51,239 = -14,826 \text{ cal/g mol} \\
&= -26,687 \text{ Btu/lb mol}
\end{align*}
\]

Assume heat of reaction is liberated in 3 h of the 4-h cycle (1/6 of an operating day):

\[
Q_r = 26,687 \left( \frac{11,145}{78.1} \right) \left( \frac{1}{6} \right) \left( \frac{1}{3} \right) -211.500 \text{ Btu/h}
\]

Use a 10°F temperature difference for the cooling water to find the mass of cooling water required to remove the heat of reaction.

\[
\text{mass of H}_2\text{O} = \frac{Q_r}{C_p \Delta T} = \frac{211.500}{(1)(10)} = 21,150 \text{ lb/h}
\]

\[
q_{\text{H}_2\text{O}} = \frac{21,150}{(60)(8.33)} = 42.3 \text{ gpm}
\]

The volumetric flow rate is, therefore, 42.3 gpm. Select a 45gpm centrifugal pump, carbon steel construction.
Equipment Design and Selection

- **HEAT TRANSFER AREA NEEDED TO COOL REACTOR**
  - Assume water inlet of 80°F with a 10°F temperature rise. A reasonable overall heat transfer coefficient for this type of heat transfer may be calculated as 45 Btu/(h ft² °F).

  \[
  \Delta T_{lm} = \frac{(115 - 80) - (115 - 90)}{2.303 \log \frac{90}{80}} = 29^\circ F
  \]

  \[
  A = \frac{Q}{U \Delta T_{lm}} = \frac{211,500}{(45)(29.7)} = 138 \text{ ft}^2
  \]

  - A 1300-gal stirred reactor has approximately 160 ft² of jacket area. Therefore, the surface area available is sufficient to maintain isothermal conditions in the reactor.

---

**SIZING OF STORAGE TANKS**

- Provide benzene and dodecane storage for six days:

  \[
  V_{benzene} = (1670)(6) = 10,020 \text{ gal}
  \]

**TABLE 1**

<table>
<thead>
<tr>
<th>Equipment specifications</th>
<th>for alkylation unit†</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. requ'd.</td>
<td>Item and description</td>
</tr>
<tr>
<td>1</td>
<td>T-1, storage tank for benzene</td>
</tr>
<tr>
<td>1</td>
<td>T-2, storage tank for dodecane</td>
</tr>
<tr>
<td>1</td>
<td>T-3, holding tank for alkylate</td>
</tr>
<tr>
<td>1</td>
<td>P-1, pump (centrifugal) for benzene transfer from T-1 to R-1</td>
</tr>
<tr>
<td>1</td>
<td>P-2, pump (centrifugal) for dodecane transfer from T-2 to R-1</td>
</tr>
<tr>
<td>1</td>
<td>P-3, pump (centrifugal) for pumping cooling water to jacket of R-1</td>
</tr>
<tr>
<td>1</td>
<td>P-4, pump (positive displacement) for alkylate transfer from T-3 to C-1</td>
</tr>
<tr>
<td>1</td>
<td>R-1, reactor (stirred) alkylator</td>
</tr>
</tbody>
</table>

†See Fig. 2-5.
Equipment Design and Selection

- The preparation of similar equipment lists for the other process units completes the equipment selection and design phase of the preliminary design.
- Figure 2-5 shows a simplified equipment diagram for the proposed process and includes the specified size or capacity of each piece of process equipment.

Economics

<table>
<thead>
<tr>
<th>TABLE 2</th>
<th>Estimated purchased-equipment cost for alkylation unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Designation</td>
<td>Item</td>
</tr>
<tr>
<td>T-1</td>
<td>Storage tank</td>
</tr>
<tr>
<td>T-2</td>
<td>Storage tank</td>
</tr>
<tr>
<td>T-3</td>
<td>Holding tank</td>
</tr>
<tr>
<td>P-1</td>
<td>Centrifugal pump (with motor)</td>
</tr>
<tr>
<td>P-2</td>
<td>Centrifugal pump (with motor)</td>
</tr>
<tr>
<td>P-3</td>
<td>Centrifugal pump (with motor)</td>
</tr>
<tr>
<td>P-4</td>
<td>Positive-displacement pump</td>
</tr>
<tr>
<td>R-4</td>
<td>Jacketed (stirred) reactor</td>
</tr>
<tr>
<td></td>
<td><strong>Total</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>TABLE 3</th>
<th>Summary of purchased-equipment cost for complete process unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Process unit</td>
<td>Purchased cost</td>
</tr>
<tr>
<td>Alkylation</td>
<td>$ 144,100</td>
</tr>
<tr>
<td>Fractionators</td>
<td>$ 175,800</td>
</tr>
<tr>
<td>Sulfonation</td>
<td>$ 245,100</td>
</tr>
<tr>
<td>Neutralization</td>
<td>$ 163,700</td>
</tr>
<tr>
<td>Spray dryer</td>
<td>$ 393,500</td>
</tr>
<tr>
<td>Auxiliary units</td>
<td>$ 142,800</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td><strong>$1,165,000</strong></td>
</tr>
</tbody>
</table>
### Economics

#### TABLE 4

<table>
<thead>
<tr>
<th>Items</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purchased equipment</td>
<td>$1,165,000</td>
</tr>
<tr>
<td>Purchased-equipment installation</td>
<td>547,600</td>
</tr>
<tr>
<td>Instrumentation and controls</td>
<td>209,700</td>
</tr>
<tr>
<td>Piping (installed)</td>
<td>768,900</td>
</tr>
<tr>
<td>Electrical (installed)</td>
<td>128,200</td>
</tr>
<tr>
<td>Buildings (including services)</td>
<td>209,700</td>
</tr>
<tr>
<td>Yard improvements</td>
<td>116,500</td>
</tr>
<tr>
<td>Service facilities (installed)</td>
<td>815,500</td>
</tr>
<tr>
<td>Land (purchase not required)</td>
<td></td>
</tr>
<tr>
<td>Engineering and supervision</td>
<td>384,500</td>
</tr>
<tr>
<td>Construction expenses</td>
<td>477,700</td>
</tr>
<tr>
<td>Contractor’s fee</td>
<td>244,700</td>
</tr>
<tr>
<td>Contingency</td>
<td>410,900</td>
</tr>
<tr>
<td>Fixed-capital investment</td>
<td>$5,557,300</td>
</tr>
<tr>
<td>Working capital</td>
<td>1,001,900</td>
</tr>
<tr>
<td>Total capital investment</td>
<td>$6,559,200</td>
</tr>
</tbody>
</table>

*Equipment cost ratio percentages used in Table 4 are factors applicable to a fluid-processing plant as outlined in Chap. 6.*

#### TABLE 5

<table>
<thead>
<tr>
<th>Items</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct production costs</td>
<td></td>
</tr>
<tr>
<td>Raw materials</td>
<td>$2,512,200</td>
</tr>
<tr>
<td>Operating labor</td>
<td>962,500</td>
</tr>
<tr>
<td>Direct supervisory and clerical labor</td>
<td>192,700</td>
</tr>
<tr>
<td>Utilities</td>
<td>567,700</td>
</tr>
<tr>
<td>Maintenance and repairs</td>
<td>111,100</td>
</tr>
<tr>
<td>Operating supplies</td>
<td>16,700</td>
</tr>
<tr>
<td>Fixed charges</td>
<td></td>
</tr>
<tr>
<td>Depreciation</td>
<td>555,700</td>
</tr>
<tr>
<td>Local taxes</td>
<td>111,100</td>
</tr>
<tr>
<td>Insurance</td>
<td>55,600</td>
</tr>
<tr>
<td>Plant-overhead costs</td>
<td>750,400</td>
</tr>
<tr>
<td>General expenses</td>
<td></td>
</tr>
<tr>
<td>Administration</td>
<td>190,100</td>
</tr>
<tr>
<td>Distribution and selling</td>
<td>773,900</td>
</tr>
<tr>
<td>Research and development</td>
<td>383,900</td>
</tr>
<tr>
<td>Financing (interest)</td>
<td>524,600</td>
</tr>
<tr>
<td>Annual total product cost</td>
<td>$7,719,200</td>
</tr>
<tr>
<td>Total product cost per pound</td>
<td>$0.515</td>
</tr>
</tbody>
</table>
Once the total product cost has been estimated, the design group is in a position to evaluate for management the attractiveness of the proposed process using such measures of profitability as rate of return, payout time, or present worth.

These methods are fully outlined in Chap. 10. The design report, as mentioned previously, completes the preliminary design.
Cost challenges for chemical engineers

- How much do we need to build a new chemical manufacturing plant?
  - estimation of capital investments

- How much does it cost to operate a chemical plant?
  - estimation of total product costs

- How can we select a “best process” from competing alternatives?
  - estimation of process profitability

Price data

- The revenues and variable costs of production are obtained by multiplying the product, feed, or utility flow rates from the flowsheet by the appropriate prices.
- The difficult step is usually finding good price data

Sources of Price Data

- Internal Company Forecasts
- Trade Journals
- Consultants
- Online Suppliers

---

1. Internal Company Forecasts

- In many large companies the marketing or planning department develops official forecasts of prices for use in internal studies.

- These forecasts sometimes include multiple price scenarios, and projects must be evaluated under every scenario. Company forecasts are occasionally made available to the public. See for example, www.Shell.com.

- When an officially approved price set exists, the design engineer should use it. The main concern is then ensuring that prices for feeds, products, or consumables that are not part of the standard forecast are put on a consistent basis.

2. Trade Journals

Several journals publish chemicals and fuel prices on a weekly basis.

- **ICIS Chemical Business Americas**, formerly known as Chemical Marketing Reporter (ICIS Publications),  [www.icispricing.com](http://www.icispricing.com)
2. Trade Journals

- **The Oil and Gas Journal** (Pennwell) publishes prices for several crude oils and a range of petroleum products on U.S., N.W. Europe, and S.E. Asia bases, as well as natural gas prices for the United States.

  ![Oil and Gas Journal](image)

- **Chemical Week** (Access Intelligence) gives prices for 22 commodity chemicals in U.S. and N.W. Europe markets.

  ![Chemical Week](image)

3. Consultants

- Companies provide information on market surveys and technical and economic analyses of competing technologies, as well as price data and forecasts on a subscription basis.

- **Purvin and Gertz**: Provides quarterly forecasts of oil, gas, and fuel prices. They have a 10-year archive of historic data and forecast prices.

  ![Purvin and Gertz](image)
3. Consultants

- Cambridge Energy Research Associates: forecasts of crude oil prices.

- Chemical Market Associates Inc. (CMAI): a large archive of historic data and future price forecasts for 70 commodity chemicals.

- SRI: The Chemical Economics Handbook series of reports published by SRI provides overviews of the markets for 281 compounds. These reports are not updated as frequently as the others but are useful for less commoditized compounds.

4. Online Suppliers

- Some caution is needed when using price data from the web. The prices quoted are generally for spot sale of small quantity orders, and are thus much higher than the market rates for large order sizes under long-term contract.

- Some prices listed online are for higher quality materials such as analytical, laboratory, or pharmaceutical grades, have much higher prices than bulk grades.
5. Reference Books

- Prices for some of the more common commodity chemicals are sometimes given in process economics textbooks.

- These prices are usually single data points rather than forecasts. They are suitable only for undergraduate design projects.

Forecasting Prices

- In most cases, it will take between 1 and 3 years for a project to go through the phases of design, procurement, and construction before a plant can begin operation.

- The plant will then operate for the project life of 10 to 20 years.

- The design engineer thus needs to carry out the economic analysis using prices forecasted over the next 20 or so years rather than the current price when the design is carried out.
Forecasting Prices

- For some compounds the only variation in price over time is minor adjustments to allow for inflation.
  - This is the case for some specialty compounds that have relatively high prices and are not subject to competitive pressure (which tends to drive prices down).
  - Prices can also be stable if they are controlled by governments, but this is increasingly rare.

- In most cases prices are determined by feedstock prices, which are ultimately determined by fluctuations in the prices of commodity fuels and chemicals.

Forecasting Prices

- Most price forecasts are based on an analysis of historic price data. Several methods are used, as illustrated. The simplest method is to use the current price, as in Figure a, but this is unsatisfactory for most commodities.

![Graph showing price fluctuations over time](image)
Forecasting Prices

- Linear regression of past prices is a good method for capturing long-term trends (>10 years), but can give very different results depending on the start data chosen, as shown in Figure b.
- This method can be very misleading if the data set is too small.

![Graph](b)

Forecasting Prices

- Many commodity prices exhibit cyclic behavior due to the investment cycle, so in some cases nonlinear models can be used, as in Figure c.
- Unfortunately, both the amplitude and the frequency of the price peaks usually vary somewhat erratically, making it difficult to fit the cyclic price behavior with simple wave models or even advanced Fourier transform methods.

![Graph](c)
A fourth approach, illustrated in Figure 4d, is to recognize that feed and product prices are usually closely linked, since increases in feed costs are passed on to customers whenever possible via increases in product price.

\[
\text{Gross margin} = \text{Revenues} - \text{Raw materials costs}
\]

Although feed and product prices may both be variable, the gross margin is therefore subject to much less variation and can be forecasted more reliably.

Forecasting of margins is the method used widely in the fuels and petrochemicals industry.

The drawbacks of this method are that it does not work very well when there are multiple routes to the same product.

In cases in which the feed prices rise rapidly, there is a drop in margins while producers wait for the market to absorb the impact of higher prices.
Forecasting Prices

- Another method is to model the statistical distribution of the price (or margin), as illustrated in Figure e.

- At its simplest, this method involves taking the average price, adjusted for inflation, over a recent period.

- This method can miss long-term trends in the data, and few prices follow any of the more commonly used distributions.

North American prices from CMAI data for polyethylene terephthalate resin (PET), which is made from terephthalic acid (TPA), which in turn is made from paraxylene (PX).

- The spot prices of PX and TPA show more volatility than the contract prices.
- All the prices follow the same broad trends.
The degree of variation in margins is clearly less than the variation in the base prices.

Simple margins for the PET value chain