UNIVERSITY OF DAIYLA

COLLEGE OF ENGINEERING

CHEMICAL ENGINEERING DEPARTMENT

CHEMICAL ENGINEERING EQUIPMENT DESIGN

For

Third and Fourth Years Chemical Engineering Students

Part -1-

Arranged by

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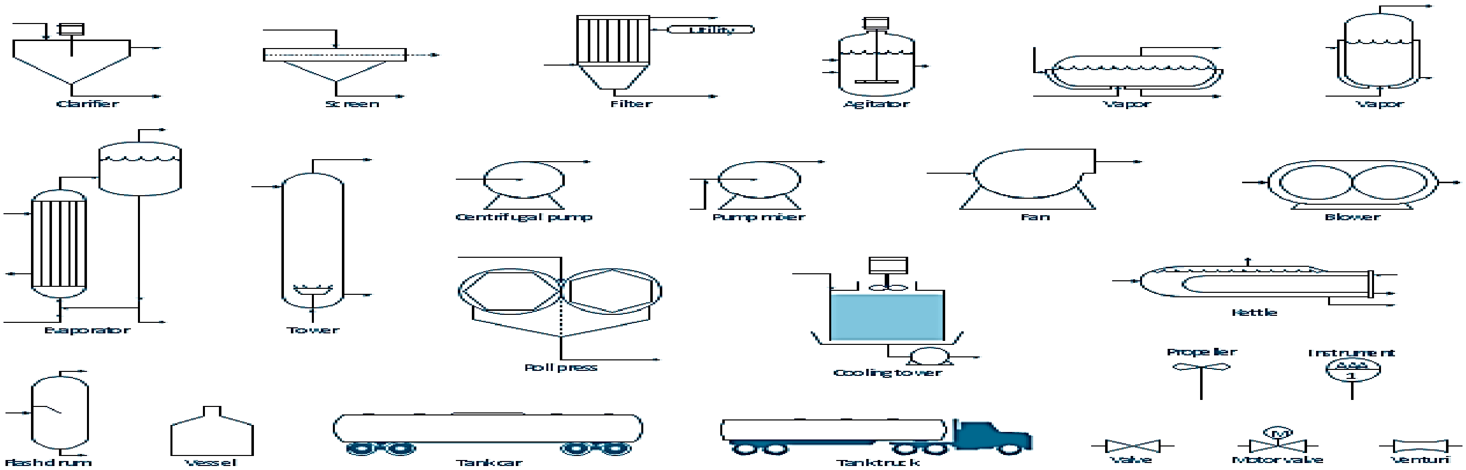
Ph.D, Ms.C and Bs.C. Chemical Engineering



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Reference books:

1. Chemical Engineering, Volume 6, Fourth edition, Chemical Engineering Design, R. K. Sinnott.
2. Plant Design and Economics for Chemical Engineers, Fourth edition, Max S. Peters, Klaus D. Timmerhaus

CHAPTER ONE

INTRODUCTION

In this modern age of industrial competition, a successful chemical engineer needs more than a knowledge and understanding of the fundamental sciences and the related engineering subjects such as thermodynamics, reaction kinetics, and computer technology. The engineer must also have the ability to apply this knowledge to practical situations for the purpose of accomplishing something that will be beneficial to society. However, in making these applications, the chemical engineer must recognize the economic implications which are involved and proceed accordingly.
Chemical engineering design of new chemical plants and the expansion or revision of existing ones require the use of engineering principles and theories combined with a practical realization of the limits imposed by industrial conditions. Development of a new plant or process from concept evaluation to profitable reality is often an enormously complex problem. A plant-design project move to completion through a series of stages such as is shown in the following:

1. Inception
2. Preliminary evaluation of economics and market
3. Development of data necessary for final design
4. Final economic evaluation
5. Detailed engineering design
6. Procurement
7. Construction
8. Startup and trial runs
9. Production

In almost every case encountered by a chemical engineer, there are several alternative methods which can be used for any given process or operation. For example, formaldehyde can be produced by catalytic t dehydrogenation of methanol, by controlled oxidation of natural gas, or by direct reaction between CO and H_2, under special conditions of catalyst, temperature, and pressure. Each of these processes contains many possible alternatives involving variables such as gas-mixture composition, temperature, pressure, and choice of catalyst. It is the responsibility of the chemical engineer, in this case, to choose the best process and to incorporate into the design the equipment and methods which will give the best results. A principle responsibility of the chemical engineer is the design, construction, and operation of chemical plants. In this responsibility, the engineer must continuously search for additional information to assist in these functions. Such information is available from numerous sources, including recent publications, operation of existing process plants, and laboratory and pilot-plant data.

Types of Designs

The methods for carrying out a design project may be divided into the following classifications, depending on the accuracy and detail required:

1. Preliminary or quick-estimate designs
2. Detailed-estimate designs

Preliminary designs are ordinarily used as a basis for determining whether further work should be done on the proposed process. The design is based on approximate process methods, and rough cost estimates are prepared. Few details are included, and the time spent on calculations is kept at a minimum. If the results of the preliminary design show that further work is justified, a *detailed-estimate design* may be developed. In this type of design, the cost and-profit potential of an established process is determined by detailed analyses and calculations.

Feasibility Survey

Before any detailed work is done on the design, the technical and economic factors of the proposed process should be examined. Following is a list of items that should be considered in making a feasibility survey:

1. Raw materials (availability, quantity, quality, cost)
2. Thermodynamics and kinetics of chemical reactions involved (equilibrium, yields, rates, optimum conditions)
3. Facilities and equipment available at present
4. Facilities and equipment which must be purchased
5. Estimation of production costs and total investment
6. Profits (probable and optimum, per pound of product and per year, return on investment)
7. Materials of construction
8. Safety considerations
9. Markets (present and future supply and demand, present uses, new uses, present buying habits, price range for products and by-products, character, location, and number of possible customers)

10. Competition (overall production statistics, comparison of various manufacturing processes, product specifications of competitors)

11**.** Properties of products (chemical and physical properties, specifications, impurities, effects of storage)

12. Sales and sales service (method of selling and distributing, advertising required, technical services required)

13. Shipping restrictions and containers

14. Plant location

15. Patent situation and legal restrictions

Equipment specifications

1. ***Columns (distillation).*** In addition to the number of plates and operating conditions it is also necessary to specify the column diameter, materials of construction, plate layout, etc.

2. ***Vessels***. In addition to size, which is often dictated by the holdup time desired materials of construction and any packing or baffling should be specified.

3. ***Reactors.*** Catalyst type and size, bed diameter and thickness, heat-interchange facilities, cycle and regeneration arrangements, materials of construction, etc., must be specified.

4. Heat exchangers and furnaces. Manufacturers are usually supplied with the duty, corrected log mean-temperature difference, percent vaporized, pressure drop desired, and materials of construction.

5. Pumps and compressors. Specify type, power requirement, pressure difference, gravities, viscosities, and working pressures.

6. Instruments. Designate the function and any particular requirement.

7. Special equipment. Specifications for mechanical separators, mixers, driers, etc.

Flow Diagrams

The chemical engineer uses flow diagrams to show the sequence of equipment and unit operations in the overall process, to simplify visualization of the manufacturing procedures, and to indicate the quantities of materials and energy transfer. These diagrams may be divided into three general types:

(1) qualitative, (2) quantitative, and (3) combined-detail.

A qualitative flow diagram indicates the flow of materials, unit operations involved, equipment necessary, and special information on operating temperatures and pressures. A quantitative flow diagram shows the quantities of materials required for the process operation. An example of a qualitative flow diagram for the production of nitric acid is shown in Fig. 2-1. Figure 2-2 presents a quantitative flow diagram for the same process.

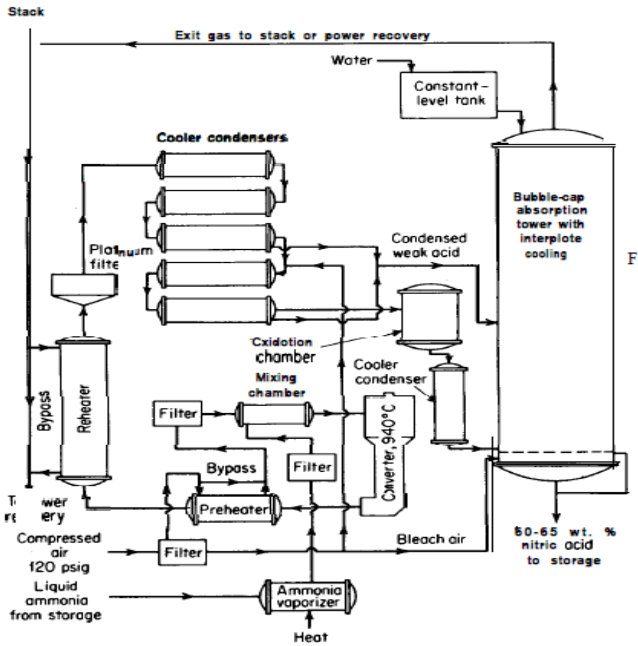


FIGURE 1 Qualitative flow diagram for the manufacture of nitric acid by the ammonia-oxidation process.

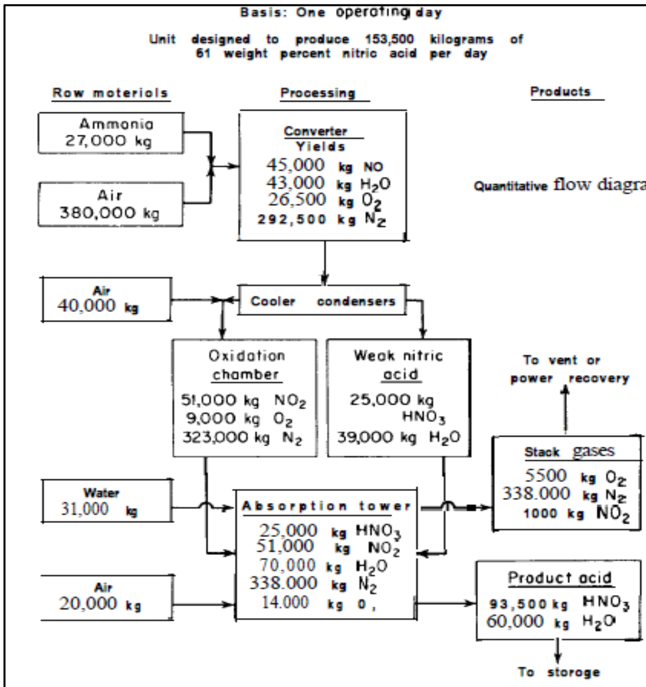


FIGURE 2

Quantitative flow diagram for the manufacture of nitric acid by the ammonia-oxidation process.

Literature Survey

A survey of the literature reveals that the majority of the nonbiodegradable detergents are alkylbenzene sulfonates (ABS). Theoretically, there are over 80,000 isomeric alkylbenzenes in the range of C,, to C,, 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. 3 for the production of sodium dodecylbenzene sulfonate.

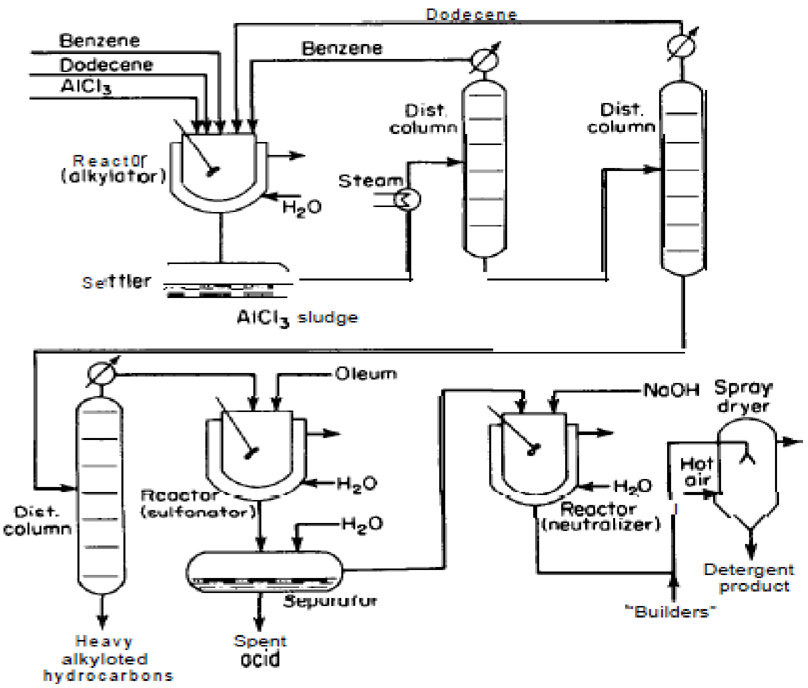


FIGURE 3
Qualitative flow diagram for the manufacture of sodium dodecylbenzene sulfonate.

A brief description of the process is as follows:

This process involves reaction of dodecene with benzene in the presence of aluminum chloride catalyst; fractionation of the resulting crude mixture to recover the desired boiling range of dodecylbenzene; sulfonation of the dodecylbenzene and subsequent neutralization of the sulfonic acid with caustic soda; blending the resulting slurry with chemical “builders”; and drying. 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. 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 SO,), 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 Na_2SO_4. 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 silitate, sodium chloride, sodium sulfate, carbovethyl 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 basic reactions which occur in the process are the following.

Alkylation:

$$C_6H_6 + C_{12}H_{24} \xrightarrow{AlCl_3} C_6H_5 \cdot C_{12}H_{25}$$

Sulfonation:

$$C_6H_5 \cdot C_{12}H_{25} + H_2SO_4 \longrightarrow C_{12}H_{25} \cdot C_6H_4 \cdot SO_3H + H_2O$$

Neutralization:

$$C_{12}H_{25} \cdot C_6H_4 \cdot SO_3H + NaOH \longrightarrow C_{12}H_{25} \cdot C_6H_4 \cdot SO_3Na + H_2O$$

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. 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. This is summarized as follows:

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.

Operating conditions for this process, as reported in the literature, vary somewhat depending upon the particular processing procedure chosen.

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 alkylator 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:

Input components:

$$\text{Product (85\% active)} = \frac{(15 \times 10^6)(0.85)}{(300)(348.5)} = 122 \text{ lb mol/day}$$

$$C_6H_6 \text{ feed} = (122)\left(\frac{1}{0.95}\right)\left(\frac{1}{0.90}\right) = 142.7 \text{ lb mol/day}$$

$$= (142.7)(78.1) = 11{,}145 \text{ lb/day}$$

$$C_{12}H_{24} \text{ feed} = 142.7 \text{ lb mol/day}$$

$$= (142.7)(168.3) = 24{,}016 \text{ lb/day}$$

$$\text{20\% oleum in} = (1.25)(11{,}145 + 24{,}016) = 43{,}951 \text{ lb/day}$$

$$\text{Dilution } H_2O \text{ in} = (0.244/1.25)(43{,}951) = 8579 \text{ lb/day}$$

$$\text{20\% NaOH in} = (1.25)(43{,}951) = 55{,}085 \text{ lb/day}$$

$$AlCl_3 \text{ catalyst in} = (0.05)(11{,}145 + 24{,}016) = 1758 \text{ lb/day}$$

Alkylation process:

$$\text{Alkylate yield} = (0.9)(142.7)(246.4) = 31{,}645 \text{ lb/day}$$

$$\text{Unreacted } C_6H_6 = (0.1)(11{,}145) = 1114 \text{ lb/day}$$

$$\text{Unreacted } C_{12}H_{24} = (0.1)(24{,}016) = 2402 \text{ lb/day}$$

Sulfur balance:

$$\text{Sulfur in} = (43{,}951)(1.045)(32.1/98.1) = 15{,}029 \text{ lb/day}$$

$$\text{Sulfur out} = \text{sulfur in detergent} + \text{sulfur in spent acid}$$

$$\text{Sulfur in detergent} = \frac{(50{,}000)(0.85)(32.1)}{(348.5)} + \frac{(50{,}000)(0.15)(32.1)}{(142)}$$

$$= 3915 + 1695 = 5610 \text{ lb/day}$$

$$\text{Sulfur out in acid} = 15{,}029 - 5610 = 9419 \text{ lb/day}$$

$$\text{Weight of 78\% } H_2SO_4 = (9419)\left(\frac{98.1}{32.1}\right)\left(\frac{1}{0.78}\right) = 36{,}861 \text{ lb/day}$$

The weight of the heavy alkylaryl hydrocarbon is obtained by difference as 3516 lb/day. The material balance summary made by the design group for the process shown in Fig. 3 is given on a daily basis in Fig. 4. After a complete material balance is made, the mass quantities are used to compute energy balances.

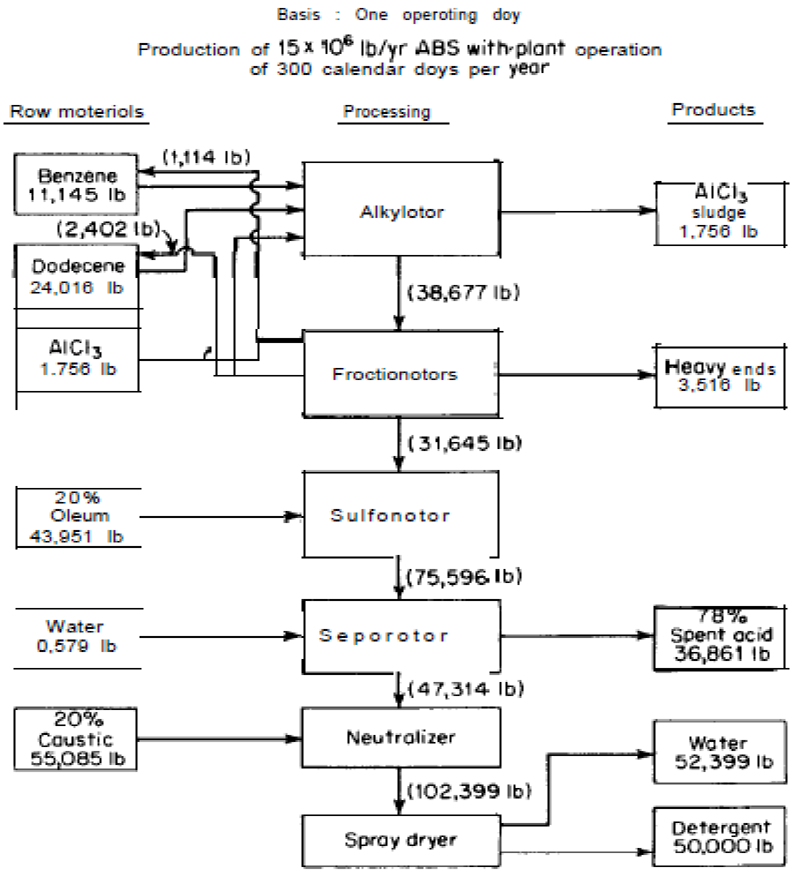


FIGURE 4
Quantitative flow diagram for the manufacture of sodium dodecylbenzene sulfonate.

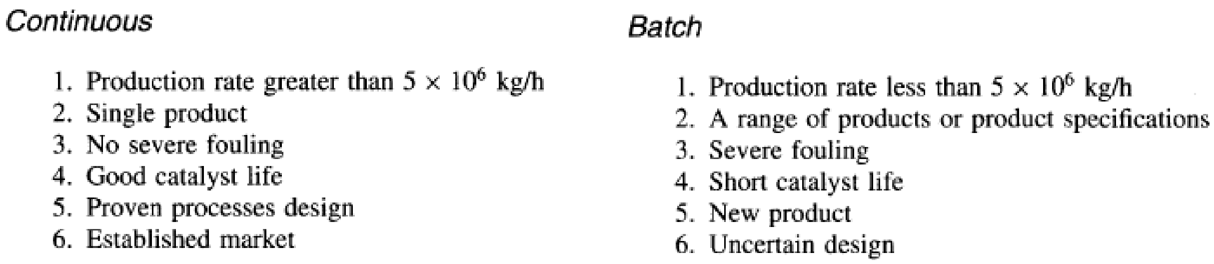
Around each piece of equipment, Temperature and pressure levels at various key points in the process, particularly at the reactors, serve as guides in making these heat balances. The complete calculations for the material and energy balances for each piece of equipment, because of their length, are not presented in this discussion.

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 to indicate the extent of the calculations which are sometimes adequate for a preliminary design.

Continuous and batch processes

Continuous processes are designed to operate 24 hours a day, 7 days a week, throughout the year. Some down time will be allowed for maintenance and, for some processes, catalyst regeneration. Batch processes are designed to operate intermittently. Some, or all, the process units being frequently shut down and started up. Continuous processes will usually be more economical for large scale production. Batch processes are used where some flexibility is wanted in production rate or product specification.

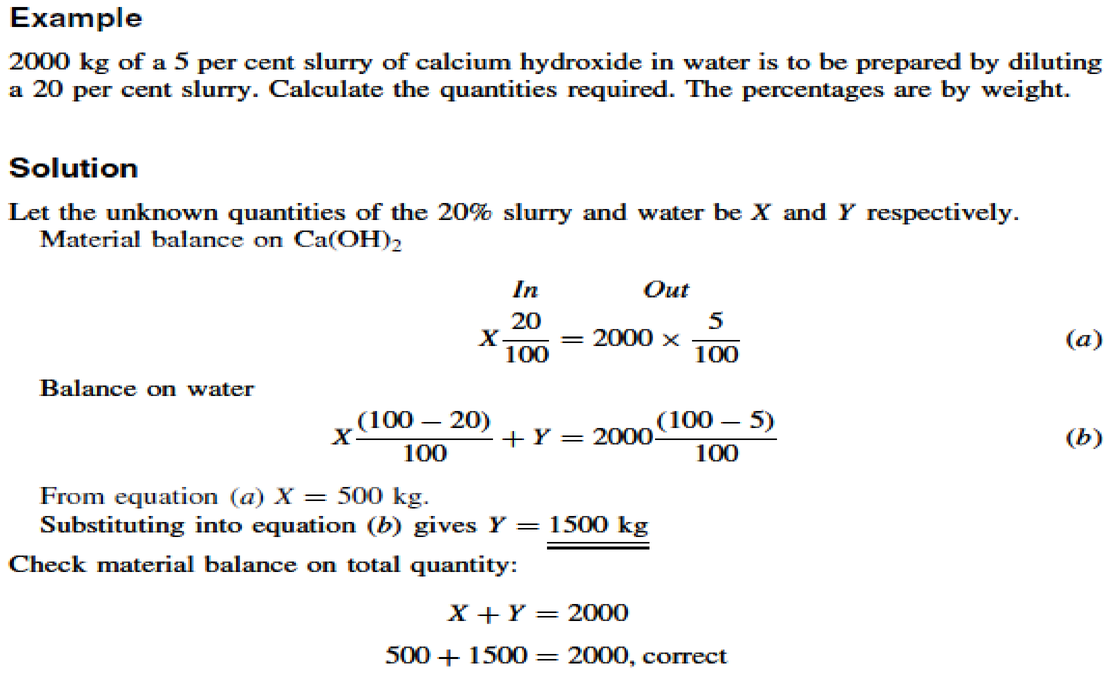


Continuous	*Batch*
1. Production rate greater than 5×10^6 kg/h	1. Production rate less than 5×10^6 kg/h
2. Single product	2. A range of products or product specifications
3. No severe fouling	3. Severe fouling
4. Good catalyst life	4. Short catalyst life
5. Proven processes design	5. New product
6. Established market	6. Uncertain design

CONSERVATION OF MASS

The general conservation equation for any process system can be written as:

Material out = Material in + Generation - Consumption – Accumulation



Example

2000 kg of a 5 per cent slurry of calcium hydroxide in water is to be prepared by diluting a 20 per cent slurry. Calculate the quantities required. The percentages are by weight.

Solution

Let the unknown quantities of the 20% slurry and water be X and Y respectively.

Material balance on $Ca(OH)_2$

$$\begin{array}{ccc} \textit{In} & & \textit{Out} \\ X\dfrac{20}{100} & = & 2000 \times \dfrac{5}{100} \end{array} \qquad (a)$$

Balance on water

$$X\frac{(100-20)}{100} + Y = 2000\frac{(100-5)}{100} \qquad (b)$$

From equation (a) $X = 500$ kg.

Substituting into equation (b) gives $Y = \underline{\underline{1500 \text{ kg}}}$

Check material balance on total quantity:

$$X + Y = 2000$$

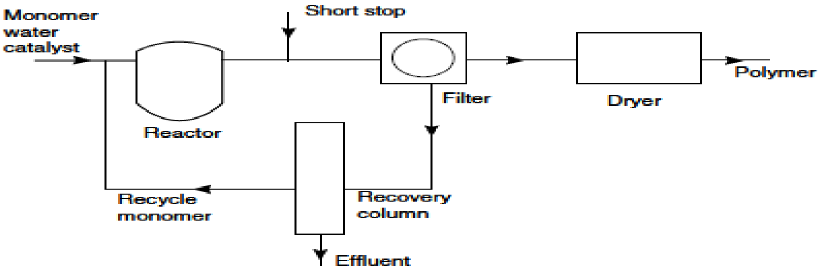
$$500 + 1500 = 2000, \text{ correct}$$

Example

Selection of system boundaries and organisation of the solution.
The diagram shows the main steps in a process for producing a polymer. From the following data, calculate the stream flows for a production rate of 10,000 kg/h.

Reactor, yield on polymer	100 per cent
slurry polymerisation	20 per cent monomer/water
conversion	90 per cent
catalyst 1 kg/1000 kg monomer	
short stopping agent	0.5 kg/1000 kg unreacted monomer

Filter, wash water approx. 1 kg/1 kg polymer
Recovery column, yield 98 per cent (percentage recovered)
Dryer, feed ~5 per cent water, product specification 0.5 per cent H_2O
Polymer losses in filter and dryer ~1 per cent

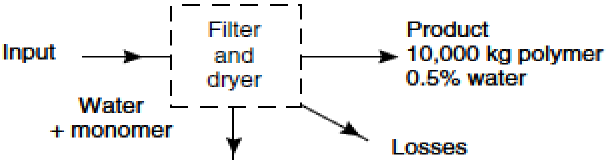


Solution

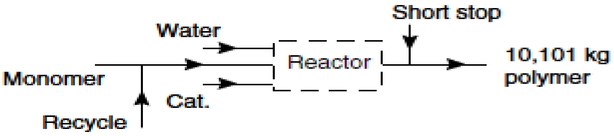
Only those flows necessary to illustrate the choice of system boundaries and method of calculation are given in the Solution.

Basis: 1 hour

Take the first system boundary round the filter and dryer.



Take the next boundary round the reactor system; the feeds to the reactor can then be calculated.



At 90 per cent conversion, monomer feed $= \dfrac{10{,}101}{0.9} = \underline{\underline{11{,}223 \text{ kg}}}$

Unreacted monomer $= 11{,}223 - 10{,}101 = \underline{\underline{1122 \text{ kg}}}$

Short-stop, at 0.5 kg/1000 kg unreacted monomer $= 1122 \times 0.5 \times 10^{-3} = \underline{\underline{0.6 \text{ kg}}}$

Catalyst, at 1 kg/1000 kg monomer $= 11{,}223 \times 1 \times 10^{-3} = \underline{\underline{11 \text{ kg}}}$

Let water feed to reactor be F_1, then for 20 per cent monomer $0.2 = \dfrac{11{,}223}{F_1 + 11{,}223}$

$$F_1 = \frac{11{,}223(1 - 0.2)}{0.2} = \underline{\underline{44{,}892 \text{ kg}}}$$

Now consider filter-dryer sub-system again.
Water in polymer to dryer, at 5 per cent (neglecting polymer loss)

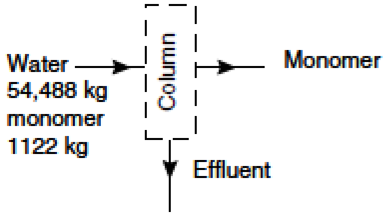
$$= 10{,}101 \times 0.05 = \underline{\underline{505 \text{ kg}}}$$

Balance over reactor-filter-dryer sub-system gives flows to recovery column.

$$\text{water, } 44{,}892 + 10{,}101 - 505 = \underline{\underline{54{,}448 \text{ kg}}}$$

$$\text{monomer, unreacted monomer, } = \underline{\underline{1122 \text{ kg}}}$$

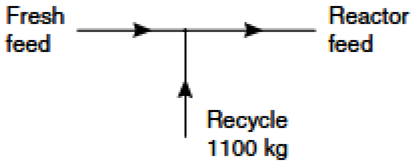
Now consider recovery system



With 98 per cent recovery, recycle to reactor

$$= 0.98 \times 1122 = \underline{\underline{1100 \text{ kg}}}$$

Composition of effluent 23 kg monomer, 54,488 kg water.
Consider reactor monomer feed



Balance round tee gives fresh monomer required

$$= 11{,}223 - 1100 = \underline{\underline{10{,}123 \text{ kg}}}$$

THE ENERGY BALANCE

Consider a steady-state process represented by Figure 5. The conservation equation can be written to include the various forms of energy.

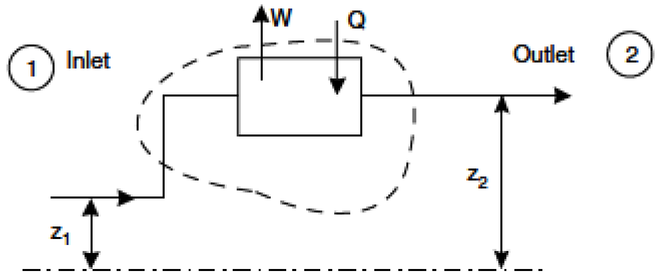


Figure 5 General steady-state process

For unit mass of material:

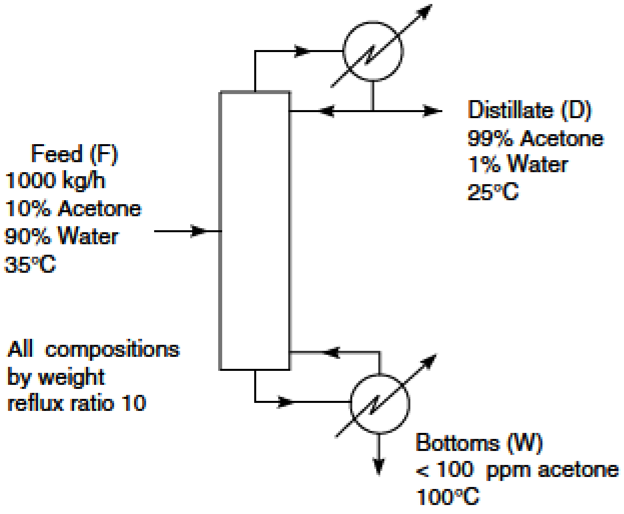
$$U_1 + P_1v_1 + u_1^2/2 + z_1g + Q = U_2 + P_2v_2 + u_2^2/2 + z_2g + W$$

$$H = U + Pv$$

The suffixes 1 and 2 represent the inlet and outlet points respectively. Q is the heat transferred across the system boundary; positive for heat entering the system, negative for heat leaving the system. W is the work done by the system; positive for work going from the system to the surroundings, and negative for work entering the system from the surroundings.

Example

Balance with no chemical reaction. Estimate the steam and the cooling water required for the distillation column shown in the figure. Steam is available at 25 psig (274 kN/m^2 abs), dry saturated. The rise in cooling water temperature is limited to 30^{0}C. Column operates at 1 bar.



Solution

Material balance

It is necessary to make a material balance to determine the top and bottoms product flow rates.

Balance on acetone, acetone loss in bottoms neglected.

$$1000 \times 0.1 = D \times 0.99$$

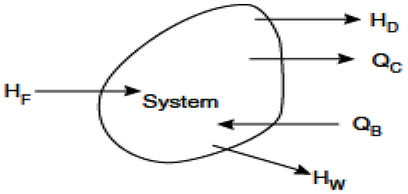
$$\text{Distillate, } D = 101 \text{ kg/h}$$

$$\text{Bottoms, } W = 1000 - 101 = 899 \text{ kg/h}$$

Energy balance

The kinetic and potential energy of the process streams will be small and can be neglected.

Take the first system boundary to include the reboiler and condenser.



Inputs: reboiler heat input Q_B + feed sensible heat H_F.

Outputs: condenser cooling Q_C + top and bottom product sensible heats $H_D + H_W$.

The heat losses from the system will be small if the column and exchangers are properly lagged (typically less than 5 per cent) and will be neglected.

Basis 25°C, 1h.

Heat capacity data, from Volume 1, average values.

Acetone:	25°C to 35°C	2.2 kJ/kg K
Water:	25°C to 100°C	4.2 kJ/kg K

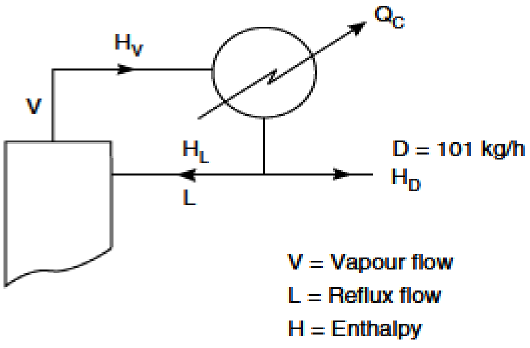
Heat capacities can be taken as additive.

Feed, 10 per cent acetone $= 0.1 \times 2.2 + 0.9 \times 4.2 = 4.00$ kJ/kg K

Tops, 99 per cent acetone, taken as acetone, 2.2 kJ/kg K

Bottoms, as water, 4.2 kJ/kg K.

Q_C must be determined by taking a balance round the condenser.



Reflux ratio (see Chapter 11, Volume 6, Chemical Engineering):

$$R = \frac{L}{D} = 10$$

$$L = 10 \times 101 = 1010 \text{ kg/h}$$

$$V = L + D = 1111 \text{ kg/h}$$

From vapor liquid equilibrium data: boiling point of 99 per cent acetone/water = 56.5°C. At steady state:

$$\text{input} = \text{output}$$

$$H_V = H_D + H_L + Q_C,$$

Hence $$Q_C = H_V - H_D - H_L$$

Assume complete condensation.

$$\text{Enthalpy of vapour } H_V = \text{latent} + \text{sensible heat.}$$

There are two ways of calculating the specific enthalpy of the vapor at its boiling point.

(1) Latent heat of vaporisation at the base temperature C sensible heat to heat the vapour to the boiling point.

(2) Latent heat of vaporisation at the boiling point C sensible heat to raise liquid to the boiling point.

Values of the latent heat of acetone and water as functions of temperature are given in Volume 1, so the second method will be used.

Latent heat acetone at 56.5^0C (330 K) = 620 kJ/kg

Water at 56.5^0C (330 K) = 2500 kJ/kg

Taking latent heats as additive:

$$H_V = 1111[(0.01 \times 2500 + 0.99 \times 620) + (56.5 - 25)2.2]$$
$$= 786{,}699 \text{ kJ/h}$$

The enthalpy of the top product and reflux are zero, as they are both at the base temperature. Both are liquid, and the reflux will be at the same temperature as the product.

Hence $$Q_C = H_V = \underline{\underline{786{,}699 \text{ kJ/h}}} \quad (218.5 \text{ kW})$$

Q_B is determined from a balance over complete system

$$\begin{array}{ccc} \text{Input} & & \text{Output} \end{array}$$

$$Q_B + H_F = Q_C + H_D + H_W$$

$$H_F = 1000 \times 4.00(35 - 25) = 40{,}000 \text{ kJ/h}$$

$$H_W = 899 \times 4.2(100 - 25) = 283{,}185 \text{ kJ/h}$$

(boiling point of bottom product taken as 100°C).

hence $$Q_B = Q_C + H_W + H_D - H_F$$
$$= 786{,}699 + 283{,}185 + 0 - 40{,}000$$
$$= \underline{\underline{1{,}029{,}884 \text{ kJ/h}}} \quad (286.1 \text{ kW})$$

Q_B is supplied by condensing steam.

$$\text{Latent heat of steam (Volume 1)} = 2174 \text{ kJ/kg at } 274 \text{ kN/m}^2$$

$$\text{Steam required} = \frac{1{,}029{,}884}{2174} = \underline{\underline{473.7 \text{ kg/h}}}$$

Q_C is removed by cooling water with a temperature rise of 30°C

$$Q_C = \text{water flow} \times 30 \times 4.2$$

$$\text{Water flow} = \frac{786{,}699}{4.2 \times 30} = \underline{\underline{6244 \text{ kg/h}}}$$

CALCULATION OF SPECIFIC ENTHALPY

For pure materials, with no phase change: $H_T = \int_{T_d}^{T} C_p \, dT$

where H_T = specific enthalpy at temperature T,
C_p = specific heat capacity of the material, constant pressure,
T_d = the datum temperature.

If a phase transition takes place between the specified and datum temperatures, the latent heat of the phase transition is added to the sensible-heat change calculated by

$$H_T = \int_{T_d}^{T_p} C_{p_1} \, dT + \int_{T_p}^{T} C_{p_2} \, dT$$

where T_p = phase transition temperature,
C_{p_1} = specific heat capacity first phase, below T_p,
C_{p_2} = specific heat capacity second phase, above T_p.

MEAN HEAT CAPACITIES

The use of mean heat capacities often facilitates the calculation of sensible-heat changes; mean heat capacity over the temperature range t_1 to t_2 is defined by the following equation:

$$C_{p_m} = \int_{t_1}^{t_2} C_p \, dt \div \int_{t_1}^{t_2} dt$$

Mean specific heat values are tabulated in various handbooks. If the values are for unit mass, calculated from some standard reference temperature, t_r, then the change in enthalpy between temperatures t_1 and t_2 is given by:

$$\Delta H = C_{p_{m,t_2}}(t_2 - t_r) - C_{p_{m,t_1}}(t_1 - t_r)$$

where t_r is the reference temperature from which the values of C_{p_m} were calculated.

If C_p is expressed as a polynomial of the form: $C_p = a + bt + ct^2 + dt^3$, then the integrated form of equation 3.14 will be:

$$C_{p_m} = \frac{a(t - t_r) + \frac{b}{2}(t^2 - t_r^2) + \frac{c}{3}(t^3 - t_r^3) + \frac{d}{4}(t^4 - t_r^4)}{t - t_r}$$

where t is the temperature at which C_{p_m} is required.

If the reference temperature is taken at 0°C, equation reduces to:

$$C_{p_m} = a + \frac{bt}{2} + \frac{ct^2}{3} + \frac{dt^3}{4}$$

and the enthalpy change from t_1 to t_2 becomes

$$\Delta H = C_{p_{m,t_2}} t_2 - C_{p_{m,t_1}} t_1$$

Note

The student must make use and review all the principles and basics of material and energy balance, units, dimensions, pressure, temperature, heat of mixing, humidity, enthalpy changes, and all information of previous years.

CHAPTER TWO
PIPING AND INSTRUMENTATION

The process flow-sheet shows the arrangement of the major pieces of equipment and their interconnection. It is a description of the nature of the process. The Piping and Instrument diagram (P and I diagram or PID) shows the engineering details of the equipment, instruments, piping, valves and fittings; and their arrangement. It is often called the Engineering Flow-sheet or Engineering Line Diagram.

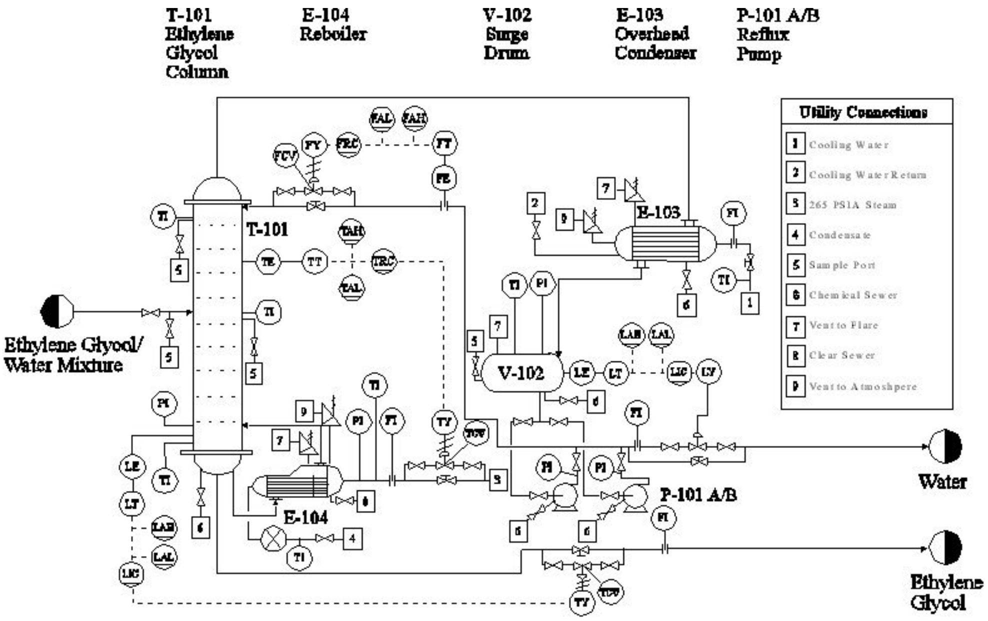
THE P AND I DIAGRAM

The P and I diagram shows the arrangement of the process equipment, piping, pumps, instruments, valves and other fittings. It should include:

1. All process equipment identified by an equipment number. The equipment should be drawn roughly in proportion, and the location of nozzles shown.
2. All pipes, identified by a line number. The pipe size and material of construction should be shown. The material may be included as part of the line identification number.
3. All valves, control and block valves, with an identification number. The type and size should be shown. The type may be shown by the symbol used for the valve or included in the code used for the valve number.
4. Ancillary fittings that are part of the piping system, such as inline sight-glasses, strainers and steam traps; with an identification number.
5. Pumps, identified by a suitable code number.
6. All control loops and instruments, with an identification number.

Symbols and layout

The symbols used to show the equipment, valves, instruments, and control loops will depend on the practice of the particular design office. The equipment symbols are usually more detailed than those used for the process flow-sheet. A typical example of a P and I diagram is shown in Figure 6. Standard symbols for instruments, controllers, and valves are given in the British Standard BS 1646.

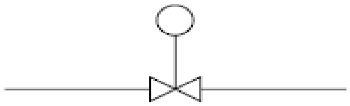


Preliminary Piping and Instrumentation Diagram for T-101

Basic symbols

The symbols illustrated below are those given in BS 1646.

Control valve



This symbol is used to represent all types of control valve, and both pneumatic and electric actuators.

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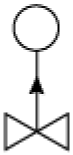
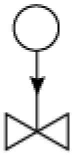
Failure mode

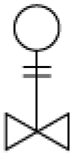
The direction of the arrow shows the position of the valve on failure of the power supply.



Fails open

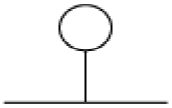


Fails shut

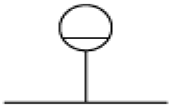


Maintains position

Instruments and controllers



Locally mounted



Main panel mounted

Locally mounted means that the controller and display is located out on the plant near to the sensing instrument location. *Main panel* means that they are located on a panel in the control room. Except on small plants, most controllers would be mounted in the control room.

Type of instrument

This is indicated on the circle representing the instrument-controller by a letter code (see Table)

Table Letter Code for Instrument Symbols (Based on BS 1646: 1979)

Property measured	First letter	Indicating only	Recording only	Controlling only	Indicating and controlling	Recording and controlling
Flow-rate	F	FI	FR	FC	FIC	FRC
Level	L	LI	LR	LC	LIC	LRC
Pressure	P	PI	PR	PC	PIC	PRC
Quality, analysis	Q	QI	QR	QC	QIC	QRC
Radiation	R	RI	RR	RC	RIC	RRC
Temperature	T	TI	TR	TC	TIC	TRC
Weight	W	WI	WR	WC	WIC	WRC
Any other property (specified in a note)	X	XI	XR	XC	XIC	XRC

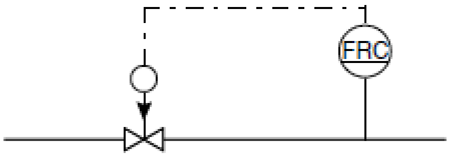
The first letter indicates the property measured; for example, F = flow. Subsequent letters indicate the function; for example,

I = indicating

RC = recorder controller

The suffixes E and A can be added to indicate emergency action and/or alarm functions.

The instrument connecting lines should be drawn in a manner to distinguish them from the main process lines. Dotted or cross-hatched lines are normally used.

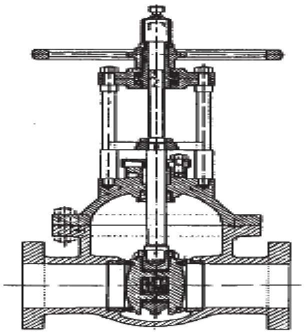


A typical control loop

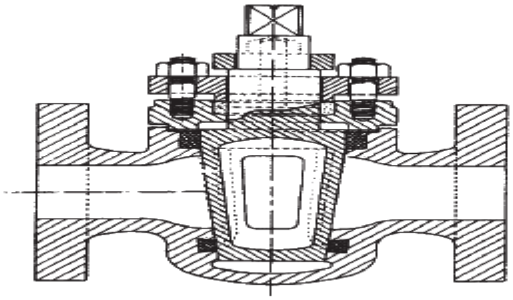
VALVE SELECTION

The valves used for chemical process plant can be divided into two broad classes, depending on their primary function:

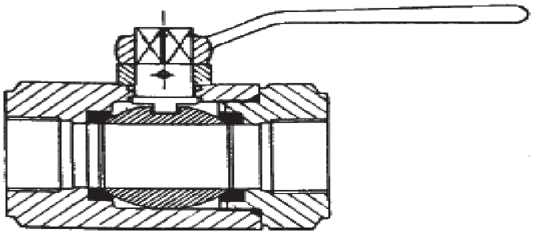
1. Shut-off valves (block valves), whose purpose is to close off the flow.
2. Control valves, both manual and automatic, used to regulate flow.



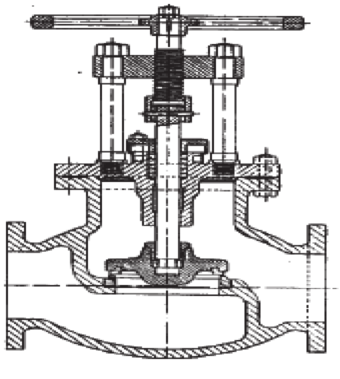
(a)



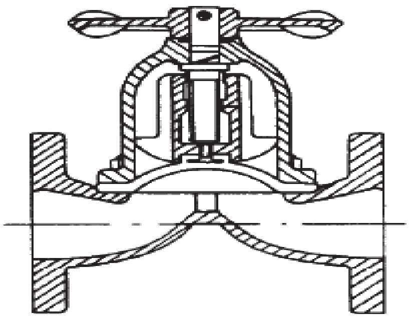
(b)



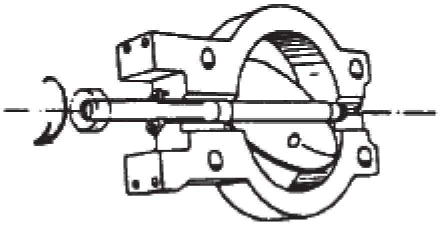
(c)



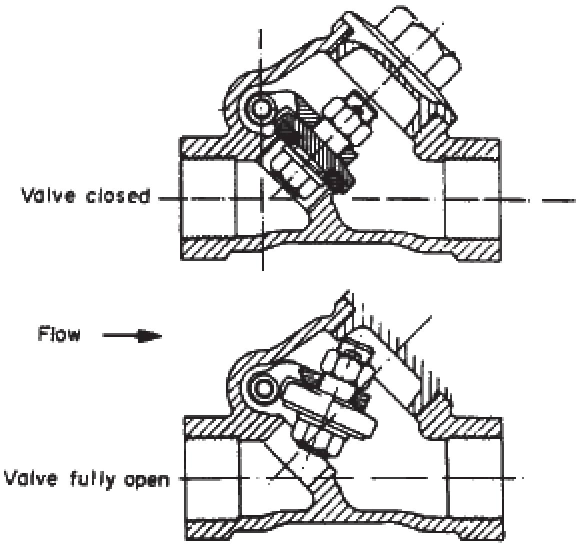
(d)



(e)



(f)



(g)

The main types of valves used are:

a. Gate
b. Plug
c. Ball
d. Globe
e. Diaphragm
f. Butterfly
g. Non-return valve

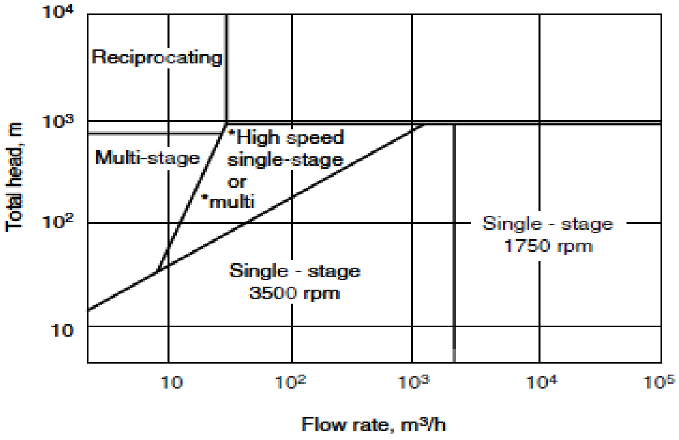
A valve selected for shut-off purposes should give a positive seal in the closed position and minimum resistance to flow when open. Gate, plug, and ball valves are most frequently used for this purpose. If flow control is required, the valve should be capable of giving smooth control over the full range of flow, from fully open to closed. Globe valves are normally used, though the other types can be used. Butterfly valves are often used for the control of gas and vapour flows. The careful selection and design of control valves is important; good flow control must be achieved, whilst keeping the pressure drop as low as possible. The valve must also be sized to avoid the flashing of hot liquids and the super-critical flow of gases and vapours. Non-return valves are used to prevent back-flow of fluid in a process line. They do not normally give an absolute shut-off of the reverse flow. A typical design is shown in Figure g.

Pump and pump selection

Pumps can be classified into two general types:

1. Dynamic pumps, such as centrifugal pumps.
2. Positive displacement pumps, such as reciprocating and diaphragm pumps.

The single-stage, horizontal, overhung, centrifugal pump is by far the most commonly used type in the chemical process industry. Other types are used where a high head or other special process considerations are specified. Pump selection is made on the flow rate and head required, together with other process considerations, such as corrosion or the presence of solids in the fluid. The chart shown in Figure below can be used to determine the type of pump required for a particular head and flow rate.



Centrifugal pump selection guide. *Single-stage >1750 rpm, multi-stage 1750 rpm

Centrifugal pumps are characterized by their specific speed. In the dimensionless form, specific speed is given by:

$$N_s = \frac{NQ^{1/2}}{(gh)^{3/4}}$$

where N = revolutions per second,
Q = flow, m^3/s,
h = head, m,
g = gravitational acceleration m/s^2.

Pump manufacturers do not generally use the dimensionless specific speed, but define it by the equation:

$$N'_s = \frac{NQ^{1/2}}{h^{3/4}}$$

where N'_s = revolutions per minute (rpm),
Q = flow, US gal/min,
h = head, ft.

$$N'_s = 1.73 \times 10^4 \; N_s$$

The specific speed for centrifugal pumps (N_s`) usually lies between 400 and 10,000, depending on the type of impeller. Generally, pump impellers are classified as radial for specific speeds between 400 and 1000, mixed flow between 1500 and 7000, and axial above 7000. Positive displacement, reciprocating, pumps are normally used where a high head is required at a low flow-rate.

Pressure drop in pipelines

The pressure drop in a pipe, due to friction, is a function of the fluid flow-rate, fluid density, and viscosity, pipe diameter, pipe surface roughness, and the length of the pipe. It can be calculated using the following equation:

$$\Delta P_f = 8f(L/d_i)\frac{\rho u^2}{2}$$

where ΔP_f = pressure drop, N/m^2, f = friction factor, L = pipe length, m, d_i = pipe inside diameter, m, ρ = fluid density, kg/m^3, u = fluid velocity, m/s.

The friction factor is a dependent on the Reynolds number and pipe roughness. The friction factor for use in equation can be found from Figure

The Renolds number is given by $Re = (\rho \times u \times d_i)/\mu$

Values for the absolute surface roughness of commonly used pipes are given in Table The parameter to use with Figure is the relative roughness, given by:

relative roughness, e = absolute roughness/pipe inside diameter

Note: the friction factor used in equation is related to the shear stress at the pipe wall, R, by the equation $f = (R/\rho u^2)$. Other workers use different relationships. Their charts for friction factor will give values that are multiples of those given by Figure . So, it is important to make sure that the pressure drop equation used matches the friction factor chart.

Table Pipe roughness

Material	Absolute roughness, mm
Drawn tubing	0.0015
Commercial steel pipe	0.046
Cast iron pipe	0.26
Concrete pipe	0.3 to 3.0

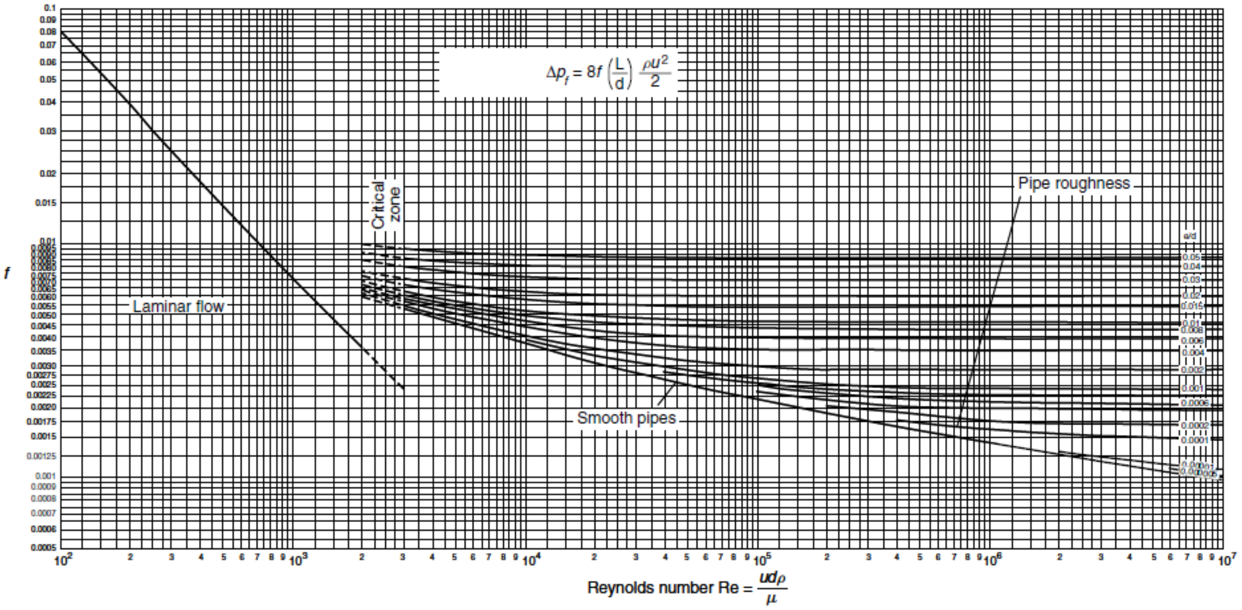


Figure Pipe friction versus Reynolds number and relative roughness

Non-Newtonian fluids

In equation and when calculating the Reynolds number for use with Figure , the fluid viscosity and density are taken to be constant. This will be true for Newtonian liquids but not for non-Newtonian liquids, where the apparent viscosity will be a function of the shear stress.

More complex methods are needed to determine the pressure drop of non-Newtonian fluids in pipelines.

There will also be a pressure drop due to the valves used to isolate equipment and control the fluid flow. The pressure drop due to these miscellaneous losses can be estimated using either of two methods:

1. As the number of velocity heads, K, lost at each fitting or valve.
   A velocity head is $u^2/2g$, metres of the fluid, equivalent to $(u^2/2)\rho$, N/m^2. The total number of velocity heads lost due to all the fittings and valves is added to the pressure drop due to pipe friction.
2. As a length of pipe that would cause the same pressure loss as the fitting or valve. As this will be a function of the pipe diameter, it is expressed as the number of equivalent pipe diameters. The length of pipe to add to the actual pipe length is found by multiplying the total number of equivalent pipe diameters by the diameter of the pipe being used.

The number of velocity heads lost, or equivalent pipe diameter, is a characteristic of the particular fitting or type of valve used. Values can be found in handbooks and manufacturers' literature. The values for a selected number of fittings and valves are given in Table

Table Pressure loss in pipe fittings and valves (for turbulent flow)

Fitting or valve	K, number of velocity heads	number of equivalent pipe diameters
45° standard elbow	0.35	15
45° long radius elbow	0.2	10
90° standard radius elbow	0.6–0.8	30–40
90° standard long elbow	0.45	23
90° square elbow	1.5	75
Tee-entry from leg	1.2	60
Tee-entry into leg	1.8	90
Union and coupling	0.04	2
Sharp reduction (tank outlet)	0.5	25
Sudden expansion (tank inlet)	1.0	50
Gate valve		
fully open	0.15	7.5
1/4 open	16	800
1/2 open	4	200
3/4 open	1	40
Globe valve, bevel seat-		
fully open	6	300
1/2 open	8.5	450
Plug valve - open	0.4	18

Example

A pipeline connecting two tanks contains four standard elbows, a plug valve that is fully open, and a gate valve that is half open. The line is commercial steel pipe, 25 mm internal diameter, length 120 m. The properties of the fluid are: viscosity 0.99 mNM^{-2} s, density 998 kg/m^3. Calculate the total pressure drop due to friction when the flow rate is 3500 kg/h.

Solution

$$\text{Cross-sectional area of pipe} = \frac{\pi}{4}(25 \times 10^{-3})^2 = 0.491 \times 10^{-3}\,\text{m}^2$$

$$\text{Fluid velocity, } u = \frac{3500}{3600} \times \frac{1}{0.491 \times 10^{-3}} \times \frac{1}{998} = 1.98\ \text{m/s}$$

$$\text{Reynolds number, } Re = (998 \times 1.98 \times 25 \times 10^{-3})/0.99 \times 10^{-3}$$
$$= 49{,}900 = 5 \times 10^4$$

Absolute roughness commercial steel pipe, Table 5.2 = 0.046 mm

Relative roughness = $0.046/(25 \times 10^{-3}) = 0.0018$, round to 0.002

From friction factor chart, Figure 5.7, $f = 0.0032$

Miscellaneous losses

fitting/valve	number of velocity heads, K	equivalent pipe diameters
entry	0.5	25
elbows	(0.8×4)	(40×4)
globe valve, open	6.0	300
gate valve, 1/2 open	4.0	200
exit	1.0	50
Total	14.7	735

Method 1, velocity heads

$$\text{A velocity head} = u^2/2g = 1.98^2/(2 \times 9.8) = 0.20 \text{ m of liquid.}$$

$$\text{Head loss} = 0.20 \times 14.7 = 2.94\ \text{m}$$

$$\text{as pressure} = 2.94 \times 998 \times 9.8 = 28{,}754\ \text{N/m}^2$$

$$\text{Friction loss in pipe, } \Delta P_f = 8 \times 0.0032 \frac{(120)}{(25 \times 10^{-3})} 998 \times \frac{1.98^2}{2}$$

$= 240{,}388\ \text{N/m}^2$ Total pressure $= 28{,}754 + 240{,}388 = 269{,}142\ \text{N/m}^2 = \underline{\underline{270\ \text{kN/m}^2}}$

Method 2, equivalent pipe diameters

Extra length of pipe to allow for miscellaneous losses

$$= 735 \times 25 \times 10^{-3} = 18.4\ \text{m}$$

So, total length for ΔP calculation $= 120 + 18.4 = 138.4$ m

$$\Delta P_f = 8 \times 0.0032 \frac{(138.4)}{(25 \times 10^{-3})} 998 \times \frac{1.98^2}{2} = 277{,}247\ \text{N/m}^2 \qquad = \underline{\underline{277\ \text{kN/m}^2}}$$

Note: the two methods will not give exactly the same result. The method using velocity heads is the more fundamentally correct approach, but the use of equivalent diameters is easier to apply and sufficiently accurate for use in design calculations.

Power requirements for pumping liquids

To transport a liquid from one vessel to another through a pipeline, energy has to be supplied to:

1. overcome the friction losses in the pipes;
2. overcome the miscellaneous losses in the pipe fittings (e.g. bends), valves, instruments etc.;
3. overcome the losses in process equipment (e.g. heat exchangers);
4. overcome any difference in elevation from end to end of the pipe;
5. overcome any difference in pressure between the vessels at each end of the pipeline.

The total energy required can be calculated from the equation:

$$g\Delta z + \Delta P/\rho - \Delta P_f/\rho - W = 0 \tag{5.5}$$

where W = work done, J/kg,
Δz = difference in elevations $(z_1 - z_2)$, m,
ΔP = difference in system pressures $(P_1 - P_2)$, N/m^2,
ΔP_f = pressure drop due to friction, including miscellaneous losses, and equipment losses, (see section 5.4.2), N/m^2,
ρ = liquid density, kg/m^3,
g = acceleration due to gravity, m/s^2.

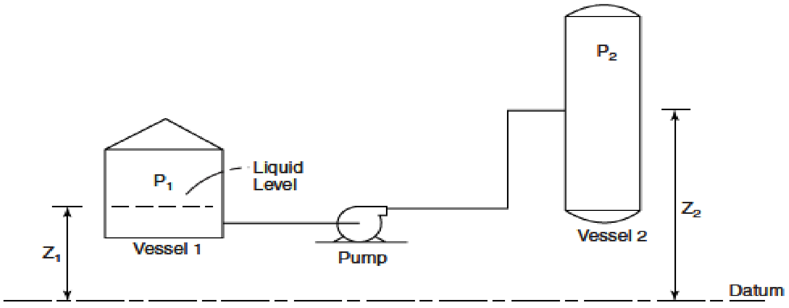


Figure 5.8. Piping system

If W is negative a pump is required; if it is positive a turbine could be installed to extract energy from the system.

$$\text{The head required from the pump} = \Delta P_f/\rho g - \Delta P/\rho g - \Delta z \tag{5.5a}$$

The power is given by:

$$\text{Power} = (W \times m)/\eta, \text{ for a pump} \tag{5.6a}$$

$$\text{and} = (W \times m) \times \eta, \text{ for a turbine} \tag{5.6b}$$

where m = mass flow-rate, kg/s,
η = efficiency = power out/power in.

The efficiency will depend on the type of pump used and the operating conditions. For preliminary design calculations, the efficiency of centrifugal pumps can be determined using Figure. 5.9.

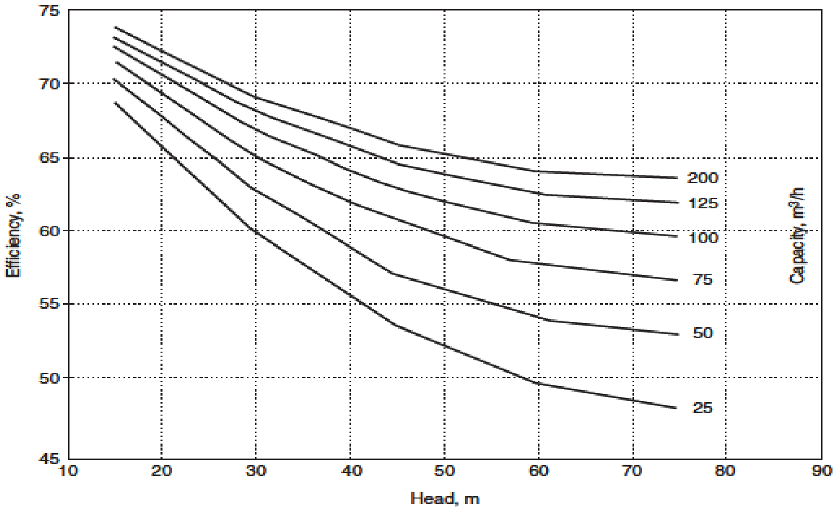


Figure 5.9. Centrifugal pump efficiency

Example

A tanker carrying toluene is unloaded, using the ship's pumps, to an on-shore storage tank. The pipeline is 225 mm internal diameter and 900 m long. Miscellaneous losses due to fittings, valves, etc., amount to 600 equivalent pipe diameters. The maximum liquid level in the storage tank is 30 m above the lowest level in the ship's tanks. The ship's tanks are nitrogen blanketed and maintained at a pressure of 1.05 bar. The storage tank has a floating roof, which exerts a pressure of 1.1 bar on the liquid. The ship must unload 1000 tonne within 5 hours to avoid demurrage charges. Estimate the power required by the pump. Take the pump efficiency as 70 per cent. Physical properties of toluene: density 874 kg/m^3, viscosity 0.62 mNm^{-2} s.

Solution

$$\text{Cross-sectional area of pipe} = \frac{\pi}{4}(225 \times 10^{-3})^2 = 0.0398\ \text{m}^2$$

$$\text{Minimum fluid velocity} = \frac{1000 \times 10^3}{5 \times 3600} \times \frac{1}{0.0398} \times \frac{1}{874} = 1.6\ \text{m/s}$$

$$\text{Reynolds number} = (874 \times 1.6 \times 225 \times 10^{-3})/0.62 \times 10^{-3}$$

$$= 507{,}484 = 5.1 \times 10^5 \qquad (5.4)$$

Absolute roughness commercial steel pipe, Table 5.2 = 0.046 mm
Relative roughness = 0.046/225 = 0.0002
Friction factor from Figure 5.7, $f = 0.0019$
Total length of pipeline, including miscellaneous losses,

$$= 900 + 600 \times 225 \times 10^{-3} = 1035\ \text{m}$$

$$\text{Friction loss in pipeline, } \Delta P_f = 8 \times 0.0019 \times \left(\frac{1035}{225 \times 10^{-3}}\right) \times 874 \times \frac{1.62^2}{2}$$

$$= \underline{\underline{78{,}221}}\ \text{N/m}^2 \qquad (5.3)$$

Maximum difference in elevation, $(z_1 - z_2) = (0 - 30) = \underline{\underline{-30\ \text{m}}}$

Pressure difference, $(P_1 - P_2) = (1.05 - 1.1)10^5 = \underline{\underline{-5 \times 10^3}}\ \text{N/m}^2$

Energy balance

$$9.8(-30) + (-5 \times 103)/874 - (78{,}221)/874 - W = 0 \qquad (5.5)$$

$$W = \underline{\underline{-389.2}}\ \text{J/kg},$$

$$\text{Power} = (389.2 \times 55.56)/0.7 = 30{,}981\ \text{W}, \quad \text{say } \underline{\underline{31\ \text{kW}}}. \qquad (5.6a)$$

MECHANICAL DESIGN OF PIPING SYSTEMS

Wall thickness: pipe schedule

The pipe wall thickness is selected to resist the internal pressure, with an allowance for corrosion. Processes pipes can normally be considered as thin cylinders; only high-pressure pipes, such as high-pressure steam lines, are likely to be classified as thick cylinders and must be given special consideration (see Chapter 13).

The British Standard 5500 gives the following formula for pipe thickness:

$$t = \frac{Pd}{20\sigma_d + P} \qquad (5.8)$$

where P = internal pressure, bar,
d = pipe od, mm,
σ_d = design stress at working temperature, N/mm^2.

Pipes are often specified by a schedule number (based on the thin cylinder formula). The schedule number is defined by:

$$\text{Schedule number} = \frac{P_s \times 1000}{\sigma_s} \qquad (5.9)$$

P_s = safe working pressure, lb/in^2 (or N/mm^2),
σ_s = safe working stress, lb/in^2 (or N/mm^2).

Schedule 40 pipe is commonly used for general purposes.

Example 5.5

Estimate the safe working pressure for a 4 in. (100 mm) dia., schedule 40 pipe, carbon steel, butt welded, working temperature 100°C. The safe working stress for butt welded steel pipe up to 120°C is 6000 lb/in^2 (41.4 N/mm^2).

Solution

$$P_s = \frac{(\text{schedule no.}) \times \sigma_s}{1000} = \frac{40 \times 6000}{1000} = \underline{\underline{240\ \text{lb/in}^2}} = \underline{\underline{1656\ \text{kN/m}^2}}$$

TYPICAL CONTROL SYSTEMS

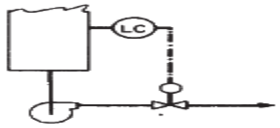


Figure 5.16. Level control

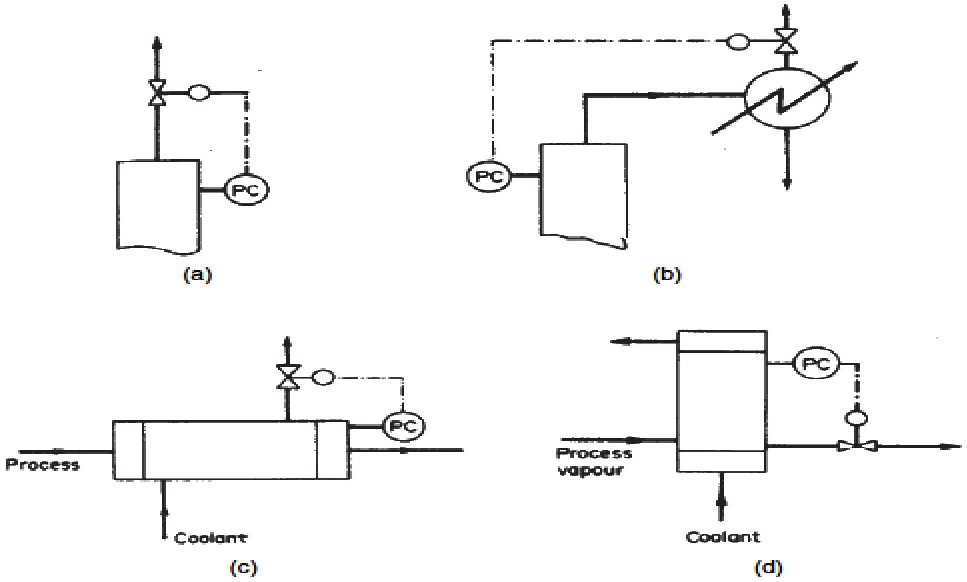


Figure 5.17. (*a*) Pressure control by direct venting (*b*) Venting of non-condensables after a condenser (*c*) Condenser pressure control by controlling coolant flow (*d*) Pressure control of a condenser by varying the heat-transfer area, area dependent on liquid level

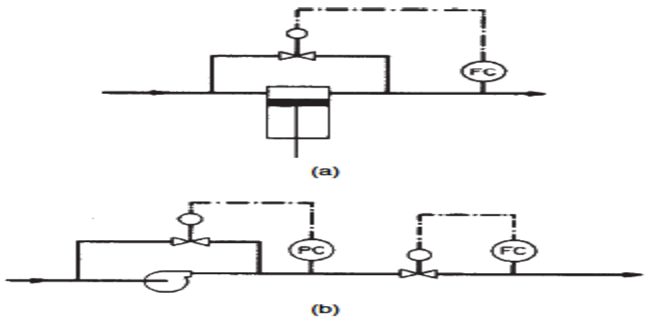


Figure 5.18. (*a*) Flow control for a reciprocating pump (*b*) Alternative scheme for a centrifugal compressor or pump

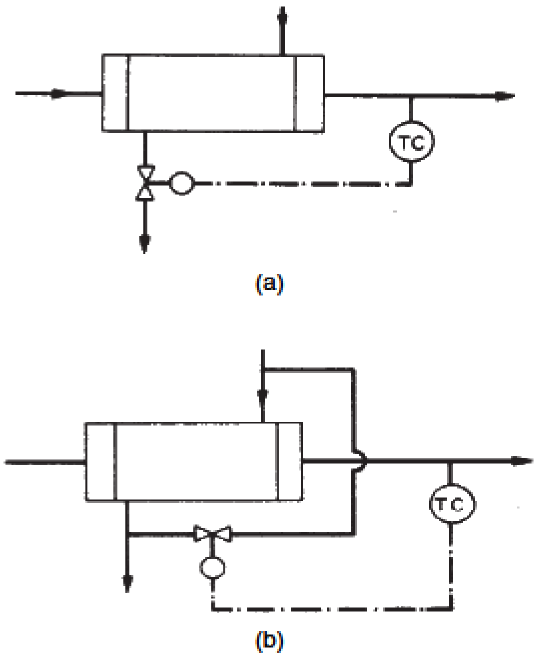


Figure 5.19. (*a*) Control of one fluid stream (*b*) By-pass control

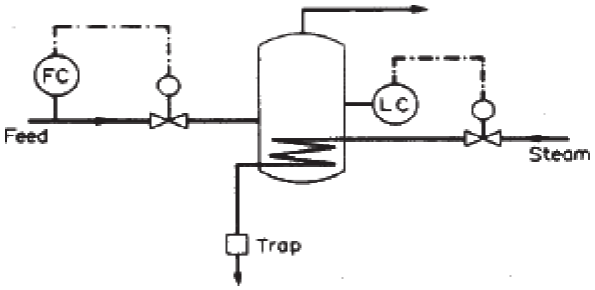


Figure 5.20. Vaporiser control

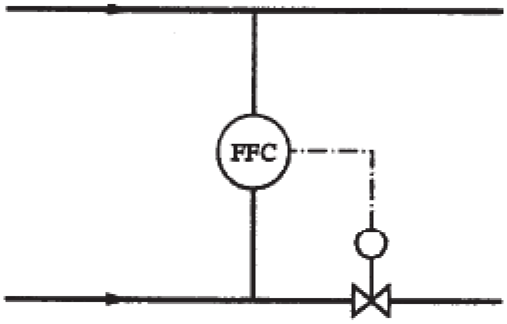


Figure 5.21. Ratio control

CHAPTER THREE
COSTING AND PROJECT EVALUATION

3.1 Costing and Project Evaluation

The design engineer needs to be able to make quick, rough, cost estimates to decide between alternative designs and for project evaluation. Chemical plants are built to make a profit, and an estimate of the investment required and the cost of production are needed before the profitability of a project can be assessed.

3.2 Accuracy and Purpose of Capital Cost Estimates

The accuracy of an estimate depends on the amount of design detail available. The accuracy of the cost data available and the time spent on preparing the estimate. Capital cost estimates can be broadly classified into three types according to their accuracy and purpose:

1. Preliminary (approximate) estimates, accuracy typically ±30 % which are used in initial feasibility studies and to make coarse choices between design alternatives.
2. Authorization (Budgeting) estimates, accuracy typically ±10 - 15 % which are used for the authorization of funds.
3. Detailed (Quotation) estimates, accuracy ±5 - 10 % which are used for project cost control and estimates for fixed price contracts.

3.3 Fixed and Working Capital

Fixed capital is the total cost of the plant ready for start-up. It is the cost paid to the contractors. It includes the cost of:

1. Design, and other engineering and construction supervision.
2. All items of equipment and their installation.
3. All piping, instrumentation and control systems.
4. Buildings and structures.
5. Auxiliary facilities, such as utilities, land and civil engineering work.

Working capital is the additional investment needed, over and above the fixed capital, to start the plant up and operate it to the point when income is earned. It includes the cost of:

1. Start-up.
2. Initial catalyst charges.

3. Raw materials and intermediates in the process.
4. Finished product inventories.
5. Funds to cover outstanding accounts from customers.

Most of the working capital is recovered at the end of the project. The total investment needed for a project is the sum of the fixed and working capital.

3.4 Cost Inflation

All cost-estimating methods use historical data, and are themselves forecasts of future costs. Some method has to be used to update old cost data for use in estimating at the design stage, and to forecast the future construction cost of the plant.

$$\text{Cost in year A} = \text{Cost in year B} \times \frac{\text{Cost index in year A}}{\text{Cost index in year B}}$$

Many methods had been adopted for estimating the values of the cost index. One is the process engineering index.

To estimate the future cost of a plant some prediction has to be made of the future annual rate of inflation. This can be based on the extrapolation of one of the published indices, tempered by the engineer's own assessment of what the future may hold.

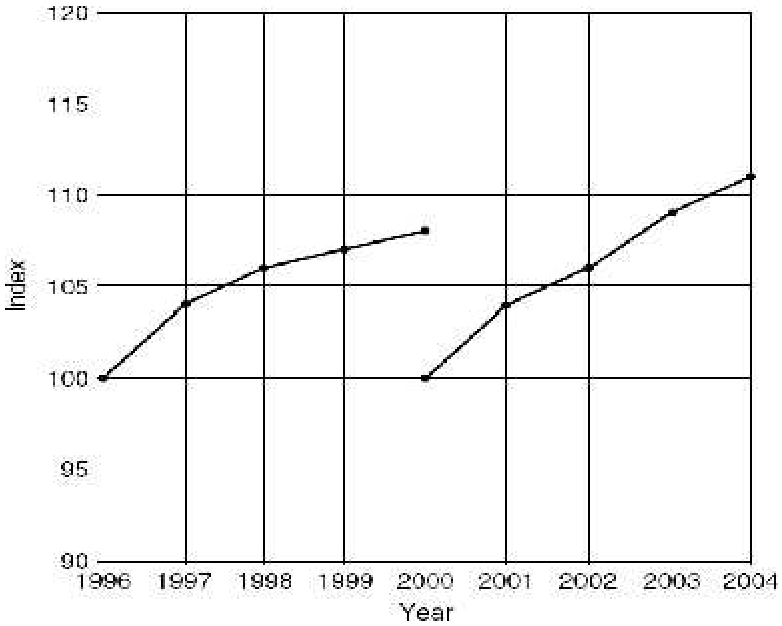


Fig. (3.1) Process Engineering Index

A composite index for the United States process plant industry is published monthly in the journal *Chemical Engineering*, the CPE plant cost index. The longer the period over which the correlation is made the more unreliable the estimate. Between 1970 and 1990 prices rose dramatically. Since then the annual rise has slowed down and is now averaging around 2 - 3 % per year.

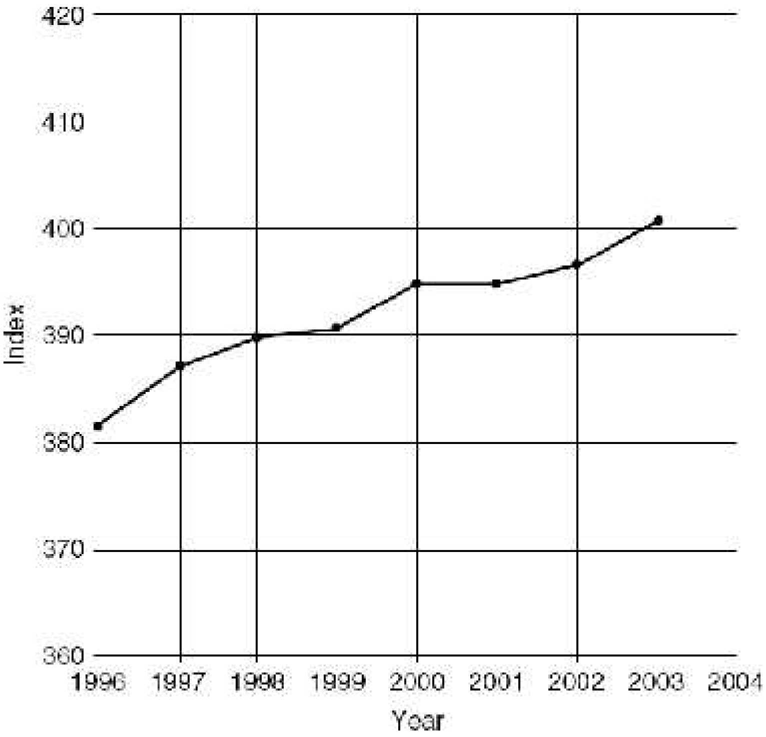


Fig. (3.2) CPE index

Example 3.1:

The purchased cost of a shell and tube heat exchanger, carbon shell, stainless steel tubes, heat transfer area 500 m^2, was £7600 in January 1998; estimate the cost in January 2006. Use the *Process Engineering* plant index.

Solution

From Process Engineering Index figure (3.1) :

Index in 1998 = 106

2000 = 108, 100 (change of base)

2004 = 111

So, estimated cost in January 2000 = 7600 × 108/106 = £7743

and in 2004 = 7743 × 111/100 = £8595

From Process Engineering Index figure (3.1):

The average increase in costs = (111-100)/4= 2.75 per year.

Use this value to predict the exchanger cost in 2006.
The cost index in 2006 = 2 × 2.75 + 111 = 116.5
Cost in 2006 = 8595 × 116.5/111 = £9021 say £9000.

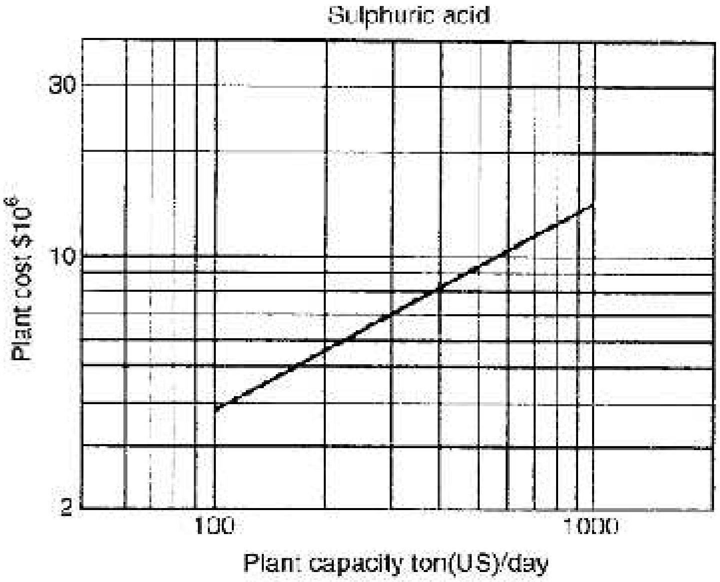
3.5 Historical Costs

An approximate estimate of the capital cost of a project can be obtained from knowledge of the cost of earlier projects using the same manufacturing process. The capital cost of a project is related to capacity by the equation

$$C_2 = C_1 \left(\frac{S_2}{S_1}\right)^n$$

Where:
C_2 = capital cost of the project with capacity, S_2
C_1 = capital cost of the project with capacity, S_1

The value of the index n is traditionally taken as 0.6; the well-known six-tenths rule. This value can be used to get a rough estimate of the capital cost if there are not sufficient data available to calculate the index for the particular process. This equation is only an approximation, and if sufficient data are available the relationship is best represented on a log-log plot. Garrett (1989) has published capital cost-plant capacity curves for over 250 processes.

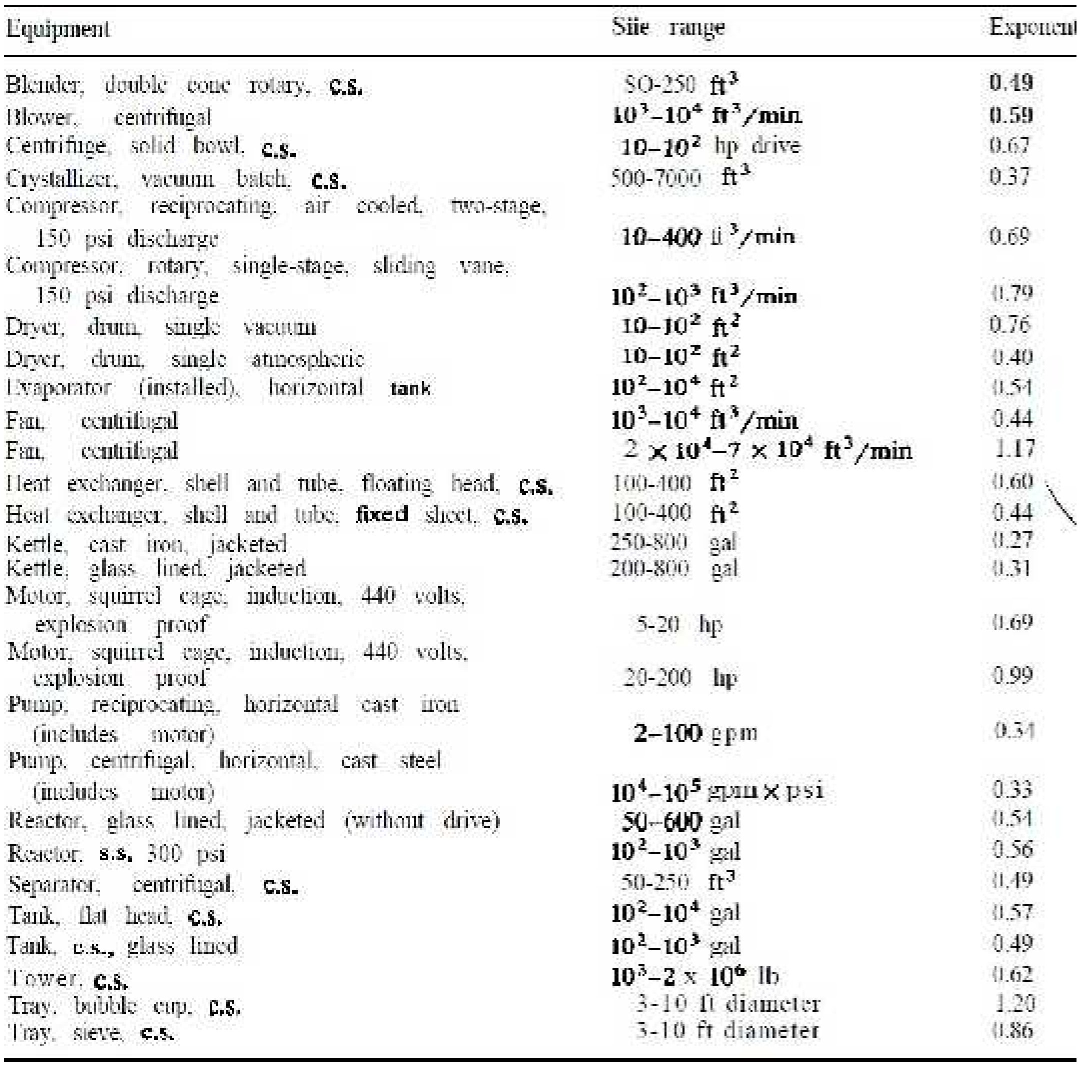


(From Garrett (1989))

3.6 Estimating Equipment Costs by Scaling

The six-tenths rule should only be used for heat exchangers in the absence of other information. In general, the cost-capacity concept should not be used beyond a tenfold range of capacity, and care must be taken to make certain the two pieces of equipment are similar with regard to type of construction, materials of construction, temperature and pressure operating range, and other pertinent variables. Table 1 contains values for other units:

Table (3.1): Typical exponents for equipment cost vs. capacity

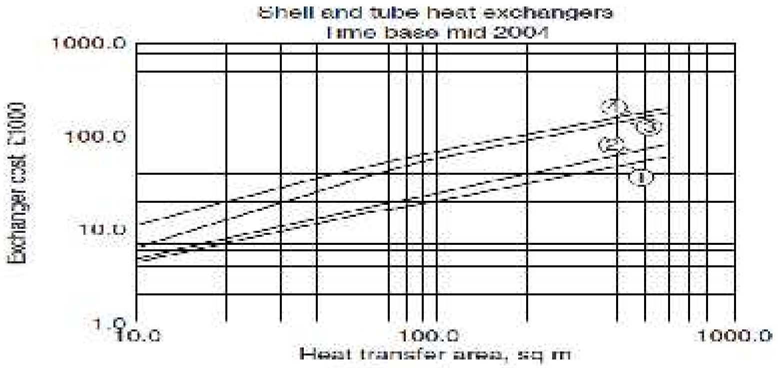


Equipment	Siie range	Exponent
Blender, double cone rotary, **c.s.**	50-250 ft^3	0.49
Blower, centrifugal	10^3–10^4 ft^3/min	0.59
Centrifuge, solid bowl, **c.s.**	10–10^2 hp drive	0.67
Crystallizer, vacuum batch, **c.s.**	500-7000 ft^3	0.37
Compressor, reciprocating, air cooled, two-stage, 150 psi discharge	10–400 ft^3/min	0.69
Compressor, rotary, single-stage, sliding vane, 150 psi discharge	10^2–10^3 ft^3/min	0.79
Dryer, drum, single vacuum	10–10^2 ft^2	0.76
Dryer, drum, single atmospheric	10–10^2 ft^2	0.40
Evaporator (installed), horizontal tank	10^2–10^4 ft^2	0.54
Fan, centrifugal	10^3–10^4 ft^3/min	0.44
Fan, centrifugal	2×10^4–7×10^4 ft^3/min	1.17
Heat exchanger, shell and tube, floating head, **c.s.**	100-400 ft^2	0.60
Heat exchanger, shell and tube, **fixed** sheet, **c.s.**	100-400 ft^2	0.44
Kettle, cast iron, jacketed	250-800 gal	0.27
Kettle, glass lined, jacketed	200-800 gal	0.31
Motor, squirrel cage, induction, 440 volts, explosion proof	5-20 hp	0.69
Motor, squirrel cage, induction, 440 volts, explosion proof	20-200 hp	0.99
Pump, reciprocating, horizontal cast iron (includes motor)	2–100 gpm	0.34
Pump, centrifugal, horizontal, cast steel (includes motor)	10^4–10^5 gpm × psi	0.33
Reactor, glass lined, jacketed (without drive)	50–600 gal	0.54
Reactor, **s.s.** 300 psi	10^2–10^3 gal	0.56
Separator, centrifugal, **c.s.**	50-250 ft^3	0.49
Tank, flat head, **c.s.**	10^2–10^4 gal	0.57
Tank, **c.s.**, glass lined	10^2–10^3 gal	0.49
Tower, **c.s.**	10^3–2×10^6 lb	0.62
Tray, bubble cup, **c.s.**	3-10 ft diameter	1.20
Tray, sieve, **c.s.**	3-10 ft diameter	0.86

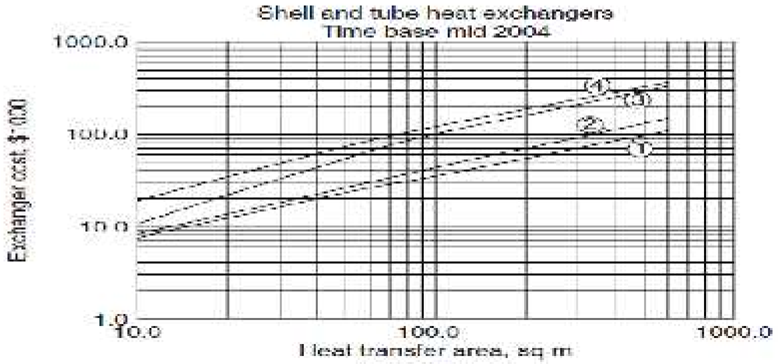
3.7 Estimation of Equipment Costs:

The cost data given in Figures (3.3) to (3.7), and Table (3.2) have been compiled from various sources. They can be used to make preliminary estimates in pounds sterling and US dollars. The base date is mid-2004, and the prices are thought to be accurate to within ±25 %.

The cost of specialized equipment, which cannot be found in the literature, can usually be estimated from the cost of the components that make up the equipment. For example, a reactor design is usually unique for a particular process but the design can be broken down into standard components (vessels, heat-exchange surfaces, agitators) the cost of which can be found in the literature and used to build up an estimate of the reactor cost.



(a) Pounds sterling



(b) US dollars

Materials

	Shell	Tubes
①	Carbon steel	Carbon steel
②	C.S.	Brass
③	C.S.	Stainless steel
④	S.S.	S.S.

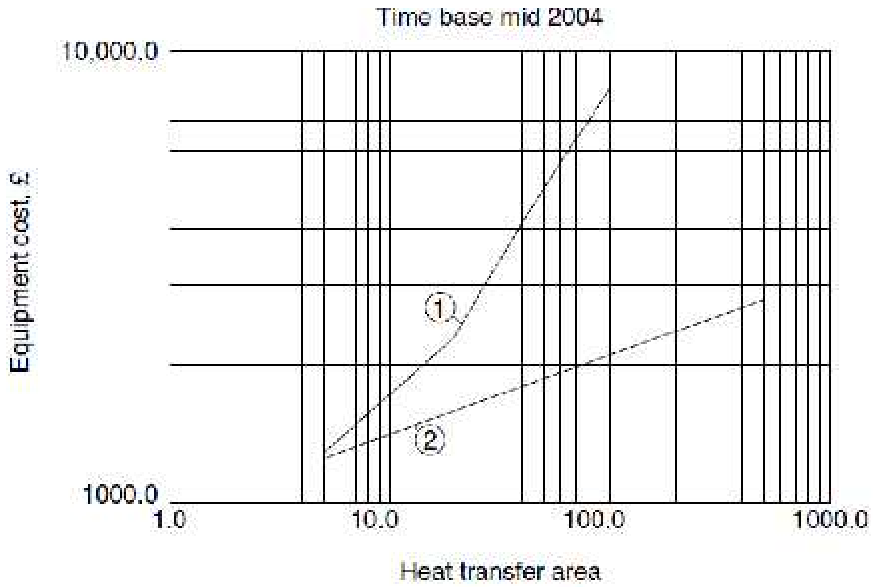
Pressure factors

1	10 bar	× 1.0
10	20	× 1.1
20	30	× 1.25
30	50	× 1.3
50	70	× 1.5

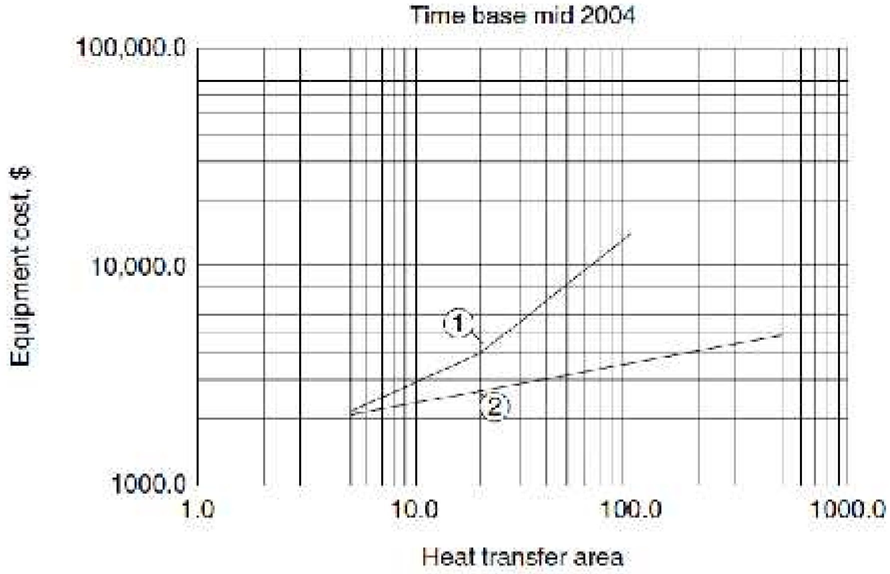
Type factors

Floating head	× 1.0
Fixed tube sheet	× 0.8
U tube	× 0.85
Kettle	× 1.3

Figure (3.3): Shell and tube heat exchangers. Time base mid-2004 Purchased cost = (bare cost from figure) × Type factor × Pressure factor.



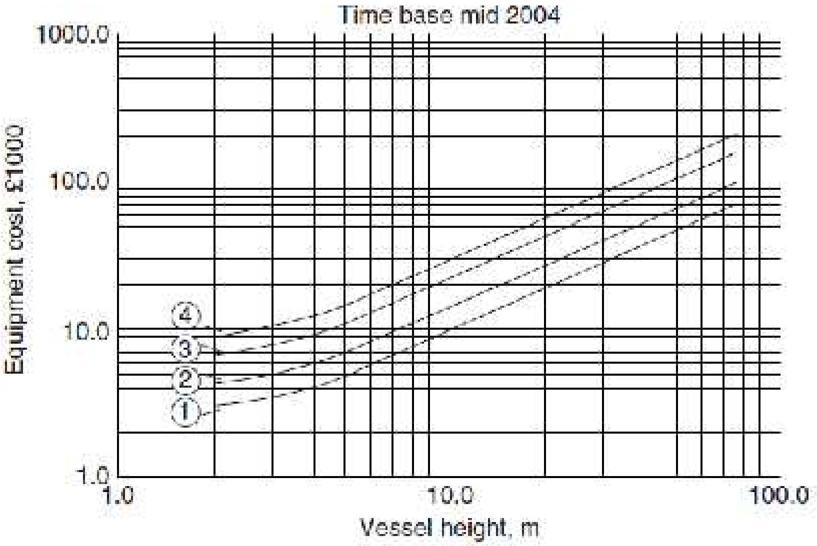
(*a*) Pounds sterling



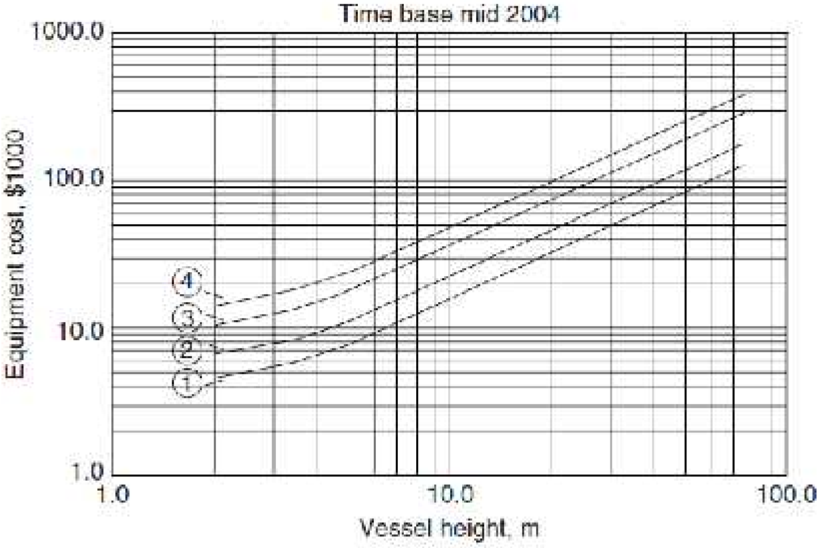
(*b*) US dollars

Type	Area scale	Material
(1) Gasketed plate	m^2	Stainless steel
(2) Double pipe	$m^2 \times 10$	Carbon steel

Figure (3.4): Gasketed plate and frame and double pipe heat exchangers, Time base mid-2004.



(*a*) Pounds sterling



(*b*) US dollars

Diameter, m			
①	0.5	③	2.0
②	1.0	④	3.0

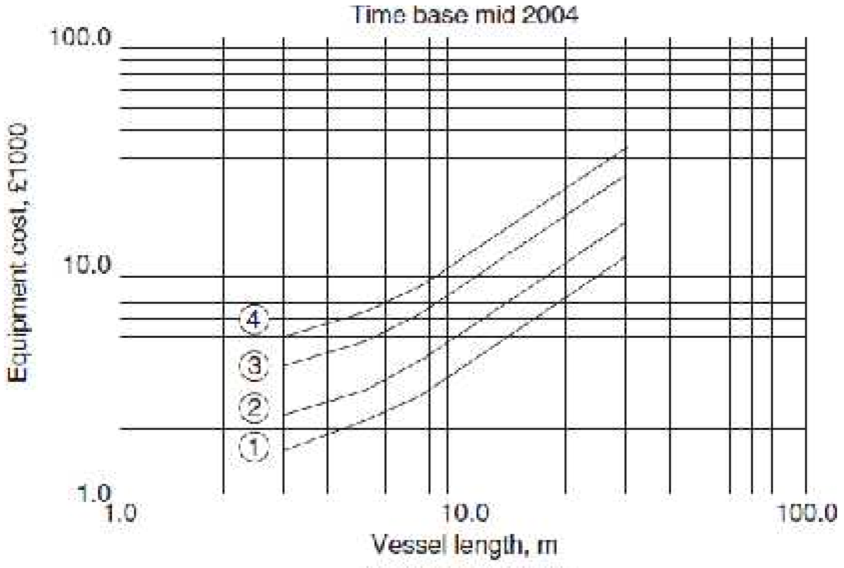
Material factors	
C.S.	× 1.0
S.S.	× 2.0
Monel	× 3.4
S.S. clad	× 1.5
Monel clad	× 2.1

Pressure factors	
1–5 bar	× 1.0
5–10	× 1.1
10–20	× 1.2
20–30	× 1.4
30–40	× 1.6
40–50	× 1.8
50–60	× 2.2

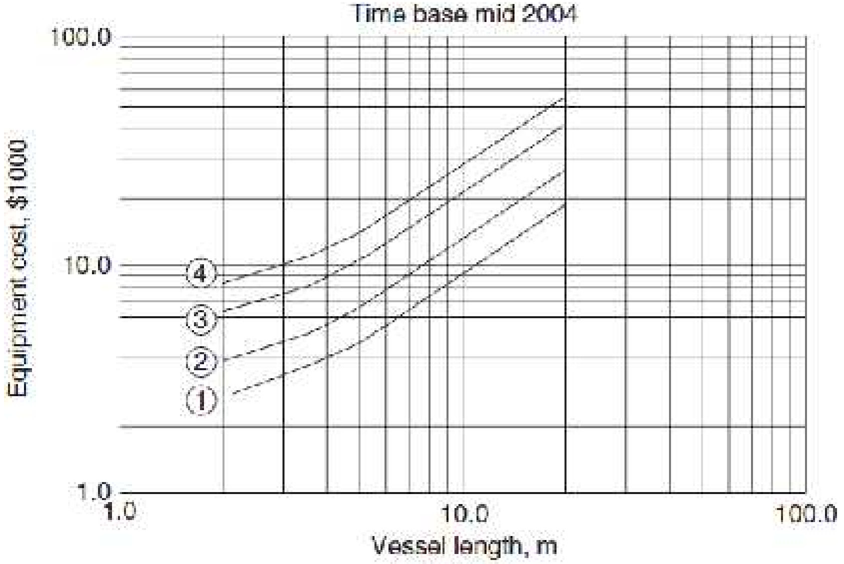
Temperature up to 300°C

Figure (3.5): Vertical pressure vessels. Time base mid-2004.

Purchased cost = (bare cost from figure) × Material factor × Pressure factor



(a) Pounds sterling



(b) US dollars

Diameter, m			
①	0.5	③	2.0
②	1.0	④	3.0

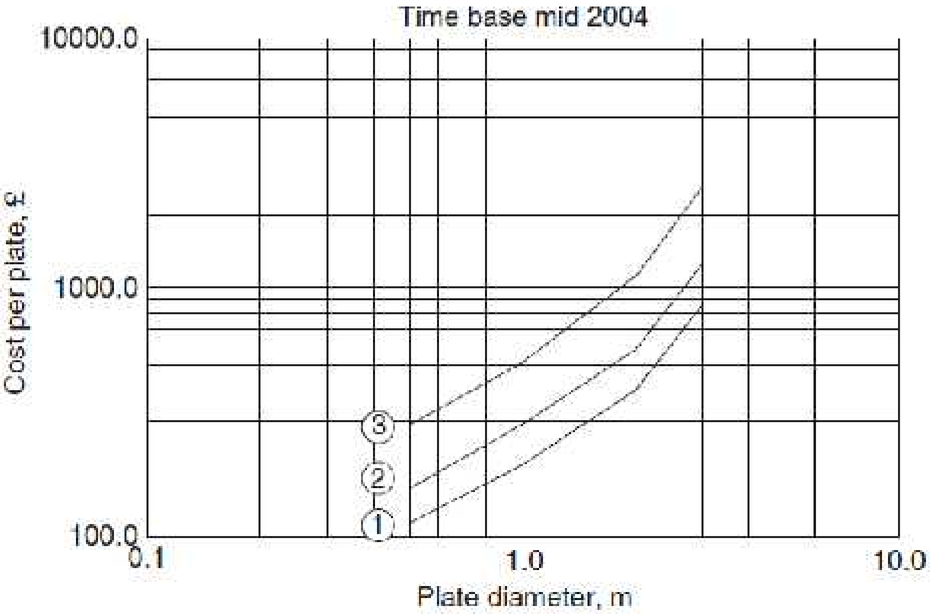
Material factors	
C.S.	× 1.0
S.S.	× 2.0
Monel	× 3.4
S.S. clad	× 1.5
Monel clad	× 2.1

Pressure factors	
1–5 bar	× 1.0
5–10	× 1.1
10–20	× 1.2
20–30	× 1.4
30 40	× 1.6
40 50	× 1.8
50 60	× 2.2

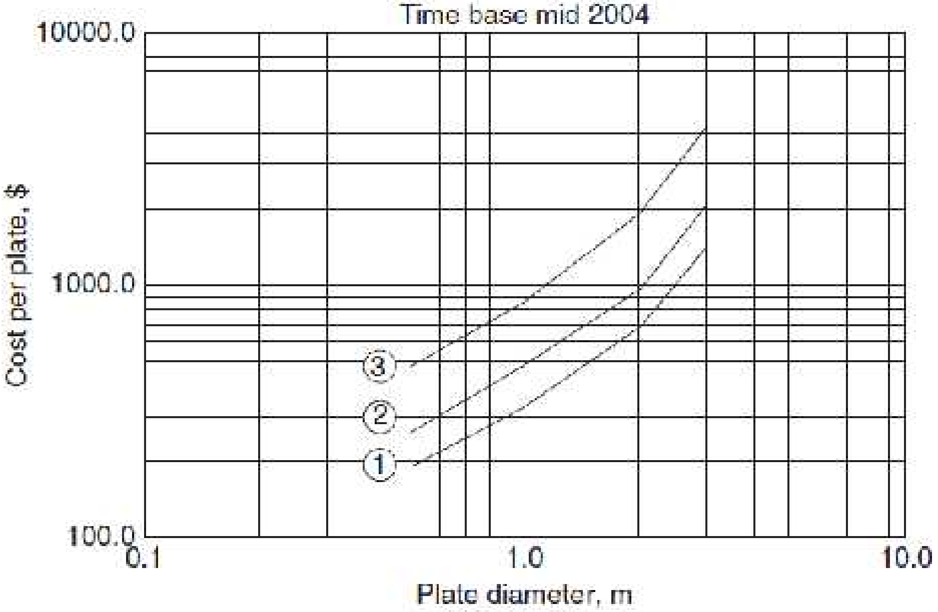
Temperature up to 300°C

Figure (3.6): Horizontal pressure vessels. Time base mid-2004.

Purchase cost = (bare cost from figure) × Material factor × Pressure factor.



(*a*) Pound sterling

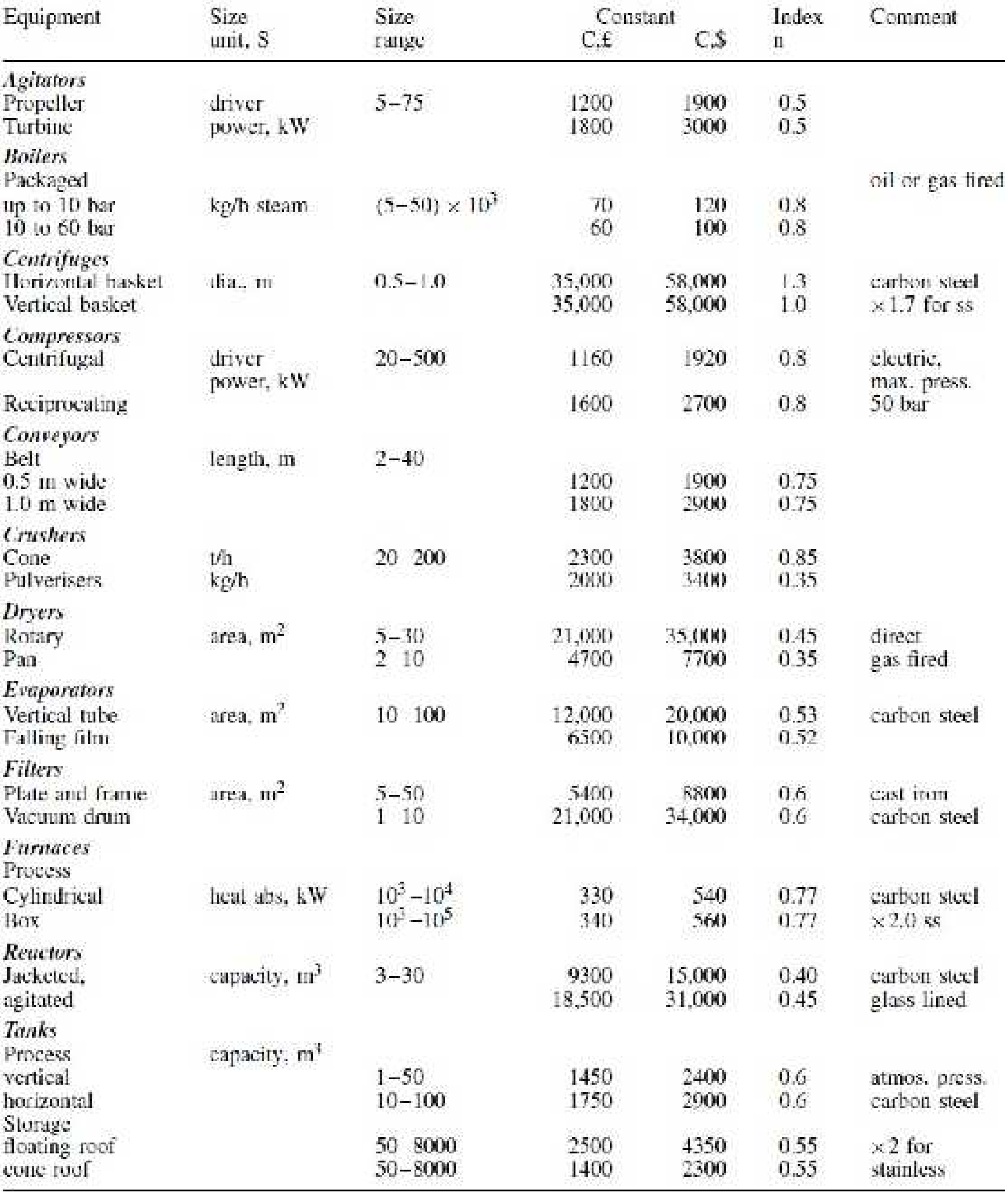


(*b*) US dollars

Type	Material factors
① Sieve	C.S. × 1.0
② Valve	S.S. × 1.7
③ Bubble cap	

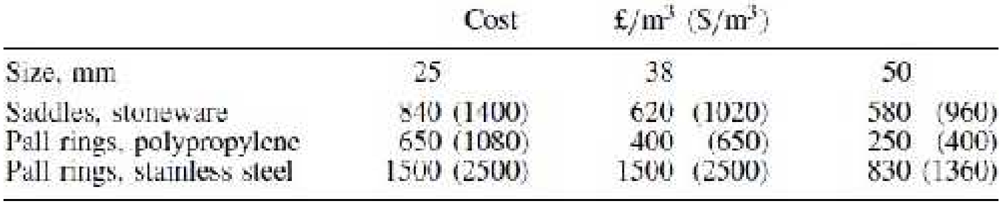
Figure (3.7): Column plates. Time base mid-2004 (for column costs see Figure 3) Installed cost = (cost from figure) × Material factor.

Table (3.2) : Cost of equipment. Cost basis mid 2004



Equipment	Size unit, S	Size range	Constant C£	Constant C$	Index n	Comment
Agitators						
Propeller	driver power, kW	5–75	1200	1900	0.5	
Turbine			1800	3000	0.5	
Boilers						
Packaged						oil or gas fired
up to 10 bar	kg/h steam	$(5-50) \times 10^3$	70	120	0.8	
10 to 60 bar			60	100	0.8	
Centrifuges						
Horizontal basket	dia., m	0.5–1.0	35,000	58,000	1.3	carbon steel
Vertical basket			35,000	58,000	1.0	×1.7 for ss
Compressors						
Centrifugal	driver power, kW	20–500	1160	1920	0.8	electric, max. press. 50 bar
Reciprocating			1600	2700	0.8	
Conveyors						
Belt	length, m	2–40				
0.5 m wide			1200	1900	0.75	
1.0 m wide			1800	2900	0.75	
Crushers						
Cone	t/h	20 200	2300	3800	0.85	
Pulverisers	kg/h		2000	3400	0.35	
Dryers						
Rotary	area, m^2	5–30	21,000	35,000	0.45	direct
Pan		2 10	4700	7700	0.35	gas fired
Evaporators						
Vertical tube	area, m^2	10 100	12,000	20,000	0.53	carbon steel
Falling film			6500	10,000	0.52	
Filters						
Plate and frame	area, m^2	5–50	5400	8800	0.6	cast iron
Vacuum drum		1 10	21,000	34,000	0.6	carbon steel
Furnaces						
Process						
Cylindrical	heat abs, kW	10^3-10^4	330	540	0.77	carbon steel
Box		10^3-10^5	340	560	0.77	×2.0 ss
Reactors						
Jacketed,	capacity, m^3	3–30	9300	15,000	0.40	carbon steel
agitated			18,500	31,000	0.45	glass lined
Tanks						
Process	capacity, m^3					
vertical		1–50	1450	2400	0.6	atmos. press.
horizontal		10–100	1750	2900	0.6	carbon steel
Storage						
floating roof		50 8000	2500	4350	0.55	×2 for
cone roof		50–8000	1400	2300	0.55	stainless

Table (3.3): Cost of column packing. Cost basis mid 2004



	Cost	£/m^3 ($/$m^3$)	
Size, mm	25	38	50
Saddles, stoneware	840 (1400)	620 (1020)	580 (960)
Pall rings, polypropylene	650 (1080)	400 (650)	250 (400)
Pall rings, stainless steel	1500 (2500)	1500 (2500)	830 (1360)

To use Table (3.2), substitute the values given for the particular type of equipment into the equation:

$$Ce = C\,S^{n}$$

where
Ce = equipment cost.
S = characteristic size parameter, in the units given in Table 2.
C = cost constant from Table (3.2).
n = index for that type of equipment.

3.7 Estimation of Total Product Cost

The cost of producing a chemical product will include the items listed below. They are divided into two groups.

Fixed costs

1. Maintenance.
2. Operating labor.
3. Laboratory costs.
4. Supervision.
5. Plant overheads.
6. Capital charges.
7. Insurance.
8. Local taxes.
9. License fees and royalty payments.

Variable costs

1. Raw materials. The prices of a selected range of chemicals are given in Table 4.
2. plant supplies.
3. Utilities (Services). Table 4 can be used to make preliminary estimates.
4. Shipping and packaging. Depend on the nature of the product.

Table (3.4): Raw material and product costs

Chemical, and state	Cost unit	Cost £/unit	Cost $/unit
Acetaldehyde, 99%	kg	0.53	0.48
Acetic acid	kg	0.60	1.10
Acetic anhydride	kg	0.70	1.15
Acetone	kg	0.63	1.03
Acrylonitrile	kg	1.20	1.90
Ally alcohol	kg	1.40	2.30
Ammonia, anhydrous	t	180	280
Ammonium nitrate, bulk	t	100	170
Ammonium sulphate, bulk	t	90	150
Amyl alcohol, mixed isomers	kg	0.67	1.20
Aniline	kg	0.52	0.84
Benzaldehyde, drums	kg	1.95	3.21
Benzene	kg	0.20	0.33
Benzoic acid, drums	kg	2.20	3.60
Butene-1	kg	0.30	0.40
n-Butyl alcohol	kg	0.75	1.30
n-Butyl ether, drums	kg	1.95	3.20
Calcium carbide, bulk	t	320	530
Calcium carbonate, bulk, coarse	t	105	145
Calcium chloride, bulk	t	200	275
Calcium hydroxide (lime), bulk	t	55	90
Carbon disulphide	t	370	500
Carbon tetrachloride, drums	kg	0.50	0.83
Chlorine	t	140	200
Chloroform	kg	0.45	0.70
Cupric chloride, anhydrous	kg	3.30	5.5
Dichlorobenzene	kg	0.95	1.54
Diethanolamine	kg	1.20	1.70
Ethanol, 90%	kg	4.20	6.50
Ethyl ether	kg	0.80	1.35
Ethylene, contract	kg	0.46	0.70
Ethylene glycol	kg	0.56	0.83
Ethylene oxide	kg	0.60	0.90
Formaldehyde, 37% w/w	kg	0.31	0.46
Formic acid, 94% w/w, drums	kg	0.63	1.05
Glycerine, 99.7%	kg	1.30	1.70
Heptane	kg	0.30	0.40
Hexane	kg	0.20	0.33
Hydrochloric acid, anhyd.	kg	1.00	1.70
Hydrochloric acid, 30% w/w	t	60	90
Hydrogen fluoride, anhydrous	kg	0.90	1.40
Hydrogen peroxide, 50% w/w	kg	0.50	0.80
Isobutanol, alcohol	kg	0.75	1.1
Isopropanol alcohol	kg	0.73	1.12
Maleic anhydride, drums	kg	1.80	2.90
Methanol	kg	0.63	1.00
Methyl ethyl ketone	kg	0.64	1.06
Monoethanolamine	kg	1.02	1.54
Methylstyrene	kg	0.70	1.15
Nitric acid, 50% w/w	t	130	220
98% w/w	t	220	370
Nitrobenzene	kg	0.47	0.78

Chemical, and state	Cost unit	Cost £/unit	Cost $/unit
Oxalic acid, sacks	kg	0.58	0.96
Phenol	kg	0.90	1.53
Phosgene, cyl.	kg	1.09	1.62
Phosphoric acid 75% w/w	kg	0.47	0.78
Potassium bicarbonate, sacks	kg	0.45	0.75
Potassium carbonate, sacks	kg	0.56	0.92
Potassium chloride	t	70	110
Potassium chromate, sacks	kg	0.80	1.30
Potassium hydroxide	kg	2.00	3.70
Potassium nitrate, bulk	t	350	570
Propylene	kg	0.43	0.64
Propylene oxide	kg	1.00	1.60
n-Propanol	kg	0.93	1.438
Sodium carbonate, sacks	kg	0.35	0.58
Sodium chloride, drums	kg	0.40	0.65
Sodium hydroxide, drums	kg	1.60	2.60
Sodium sulphate, bulk	t	72	120
Sodium thiosulphate	kg	0.38	0.57
Sulphur, crude, 99.5%, sacks	t	85	140
Sulphuric acid, 98% w/w	t	40	65
Titanium dioxide, sacks	kg	1.50	2.50
Toluene	kg	0.32	0.47
Toluene diisocyanate	kg	2.20	3.20
Trichloroethane	kg	0.56	0.94
Trichloroethylene	kg	0.84	1.40
Urea, 46% nitrogen, bulk	t	120	160
Vinyl acetate	kg	0.65	1.08
Vinyl chloride	kg	0.44	0.66
Xylenes	kg	0.29	0.43

Anhyd. = anhydrous, cyl. = cylinder, refin. = refined

Table (3.5) Cost of utilities, typical figures mid-2004

Utility	UK	USA
Mains water (process water)	60 p/t	50 c/t
Natural gas	0.4 p/MJ	0.7 c/MJ
Electricity	1.0 p/MJ	1.5 c/MJ
Fuel oil	65 £/t	100 $/t
Cooling water (cooling towers)	1.5 p/t	1 c/t
Chilled water	5 p/t	8 c/t
Demineralised water	90 p/t	90 c/t
Steam (from direct fired boilers)	7 £/t	12 $/t
Compressed air (9 bar)	0.4 p/m^3 (Stp)	0.6 c/m^3
Instrument air (9 bar) (dry)	0.6 p/m^3 (Stp)	1 c/m^3
Refrigeration	1.0 p/MJ	1.5 c/MJ
Nitrogen	6 p/m^3 (Stp)	8 c/m^3

Note: £1 = 100p, 1$ = 100c, 1 t = 1000 kg = 2200 ib, stp = 1 atm, 0°C

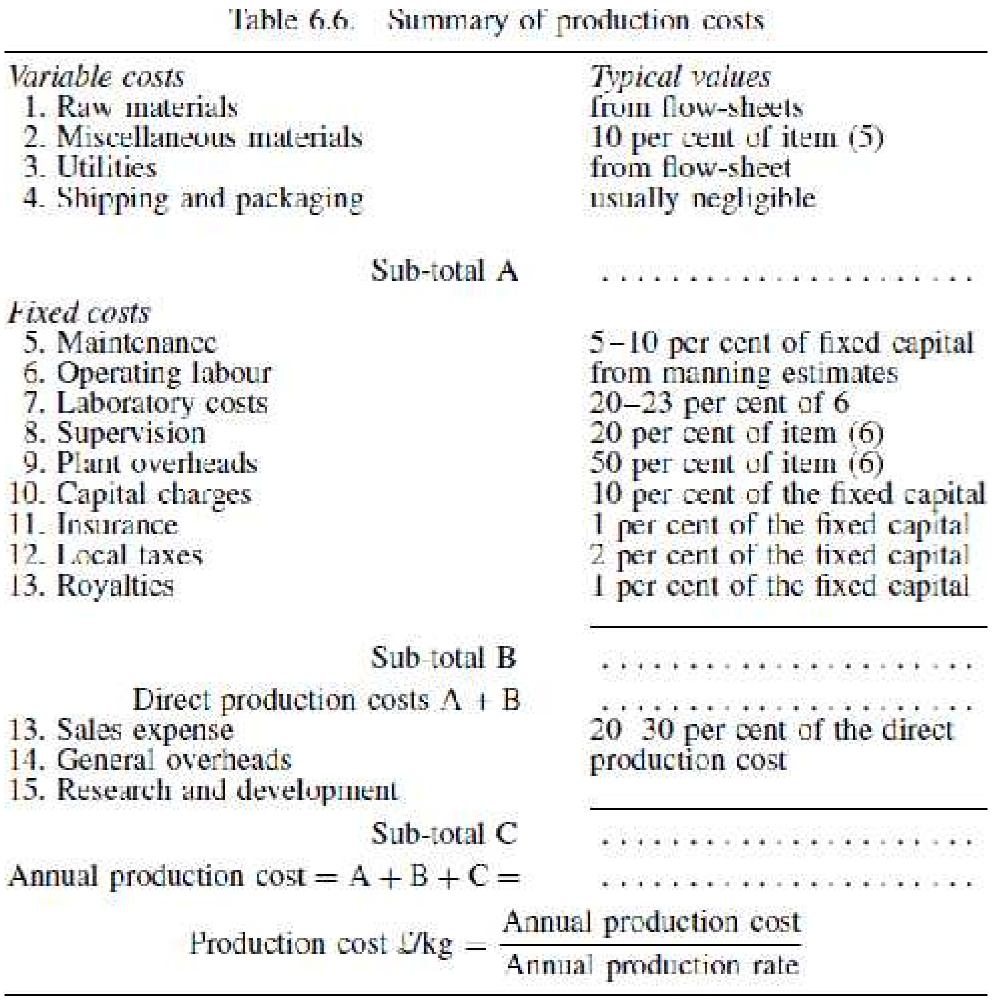


Table 6.6. Summary of production costs

Variable costs	*Typical values*
1. Raw materials	from flow-sheets
2. Miscellaneous materials	10 per cent of item (5)
3. Utilities	from flow-sheet
4. Shipping and packaging	usually negligible
Sub-total A	....
Fixed costs	
5. Maintenance	5–10 per cent of fixed capital
6. Operating labour	from manning estimates
7. Laboratory costs	20–23 per cent of 6
8. Supervision	20 per cent of item (6)
9. Plant overheads	50 per cent of item (6)
10. Capital charges	10 per cent of the fixed capital
11. Insurance	1 per cent of the fixed capital
12. Local taxes	2 per cent of the fixed capital
13. Royalties	1 per cent of the fixed capital
Sub-total B	....
Direct production costs A + B	....
13. Sales expense	20–30 per cent of the direct production cost
14. General overheads	
15. Research and development	
Sub-total C	....
Annual production cost = A + B + C =	....

$$\text{Production cost £/kg} = \frac{\text{Annual production cost}}{\text{Annual production rate}}$$

Example 3.2:

Preliminary design work has been done on a process to recover a valuable product from an effluent gas stream. The gas will be scrubbed with a solvent in a packed column; the recovered product and solvent separated by distillation; and the solvent cooled and recycled. The major items of equipment that will be required are detailed below.

1. Absorption column : diameter 1 m, vessel overall height 15 m, packed height 12m, packing 25mm ceramic intalox saddles, vessel carbon steel, operating pressure 5 bar.
2. Recovery column : diameter 1 m, vessel overall height 20 m, 35 sieve plates, vessel and plates stainless steel, operating pressure 1 bar.
3. Reboiler : forced convection type, fixed tube sheets, area 18.6 m^2, carbon steel shell, stainless-steel tubes, operating pressure 1 bar.
4. Condenser : fixed tube sheets, area 25.3 m^2, carbon steel shell and tubes, operating pressure 1 bar.

5. Recycle solvent cooler : U-tubes, area 10.1 m^2, carbon steel shell and tubes, operating pressure 5 bar.
6. Solvent storage tanks : cone roof, capacity 100 m^3, carbon steel.

Solution

Absorption column

Bare vessel cost (Figure 3.5a) £21,000; material factor 1.0, pressure factor 1.1

Vessel cost = 21,000 × 1.0 × 1.1 = £23,000

Packing cost (Table 3.3) £840/m^3

Volume of packing = $(\pi/4)\ d^2 \times L = (\pi/4) \times 12 = 9.4$

m^3 Cost of column packing = 9.4 × 840 = £7896

Total cost of column 23,000 + 7896 = 30,896 say £31,000

Recovery column

Bare vessel cost (Figure 3.5a) £26,000; material factor 2.0, pressure factor 1.0

Vessel cost 26,000 × 2.0 × 1.0 = £52,000

Cost of a plate (Figure 3.7a), material factor 1.7 = 200 × 1.7 =

£340 Total cost of plates = 35 × 340 = £11,900

Total cost of column = 52,000 + 11,900 = 63,900 say £64,000

Reboiler

Bare cost (Figure 3.3a) £11,000; type factor 0.8, pressure

factor 1.0 Purchased cost = 11,000 × 0.8 × 1.0 = £8800

Condenser

Bare cost (Figure 3.3a) £8500; type factor 0.8, pressure

factor 1.0 Purchased cost = 8500 × 0.8 × 1.0 = £6800

Cooler

Bare cost (Figure 3.3a) £4300; type factor 0.85, pressure

factor 1.0 Purchased cost = 4300 × 0.85 × 1.0 = £3700

Solvent tank

Purchase cost (Table 3.2) = $1400 \times (100)^{0.55}$ = £17625

Total purchase cost of major equipment items (PCE)

Absorption column	31,000
Recovery column	64,000
Reboiler	8,800
Condenser	6,800
Cooler	3,700
Solvent tank	17,700
Total	**£132,000**

CHAPTER FOUR
MATERIALS OF CONSTRUCTION

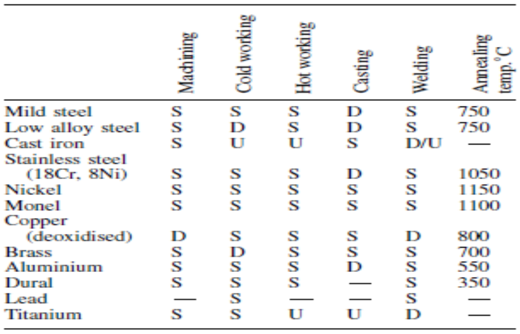
Many factors have to be considered when selecting engineering materials, but for chemical process plant the overriding consideration is usually the ability to resist corrosion. The process designer will be responsible for recommending materials that will be suitable for the process conditions.

MATERIAL PROPERTIES

The most important characteristics to be considered when selecting a material of construction are:

1. Mechanical properties
(a) Strength tensile strength
(b) Stiffness elastic modulus (Young's modulus)
(c) Toughness fracture resistance
(d) Hardness wear resistance
(e) Fatigue resistance
(f) Creep resistance
2. The effect of high and low temperatures on the mechanical properties.
3. Corrosion resistance
4. Any special properties required; such as, thermal conductivity, electrical resistance, magnetic properties
5. Ease of fabrication forming, welding, and casting (see Table 7.1)
6. Availability in standard sizes plates, sections, tubes
7. Cost.

Table 7.1. A guide to the fabrication properties of common metals and alloys



	Machining	Cold working	Hot working	Casting	Welding	Annealing temp. °C
Mild steel	S	S	S	D	S	750
Low alloy steel	S	D	S	D	S	750
Cast iron	S	U	U	S	D/U	—
Stainless steel (18Cr, 8Ni)	S	S	S	D	S	1050
Nickel	S	S	S	S	S	1150
Monel	S	S	S	S	S	1100
Copper (deoxidised)	D	S	S	S	D	800
Brass	S	D	S	S	S	700
Aluminium	S	S	S	D	S	550
Dural	S	S	S	—	S	350
Lead	—	S	—	—	S	—
Titanium	S	S	U	U	D	—

S — Satisfactory, D — Difficult, special techniques needed.
U — Unsatisfactory.

1. MECHANICAL PROPERTIES

Typical values of the mechanical properties of the more common materials used in the construction of chemical process equipment are given in Table 7.2.

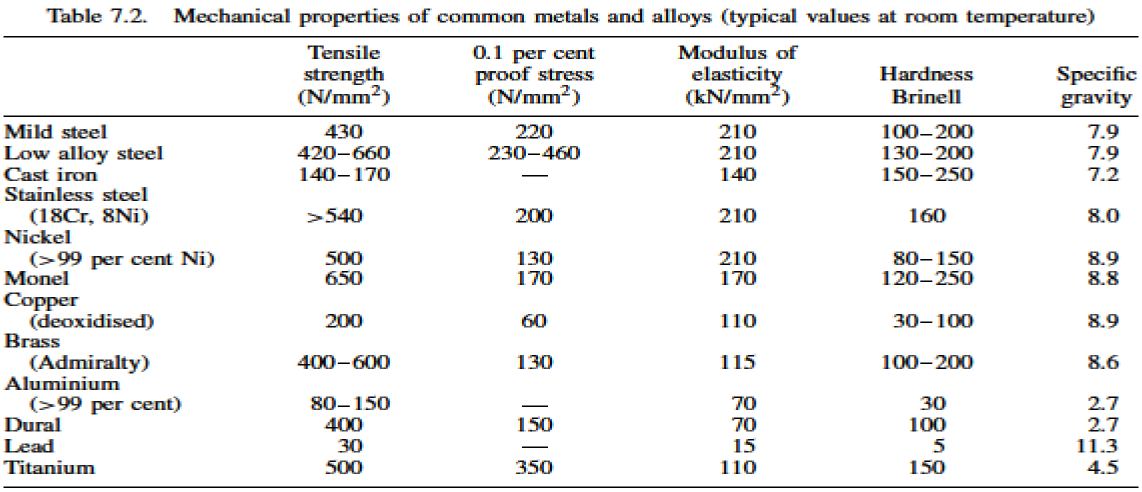


Table 7.2. Mechanical properties of common metals and alloys (typical values at room temperature)

	Tensile strength (N/mm^2)	0.1 per cent proof stress (N/mm^2)	Modulus of elasticity (kN/mm^2)	Hardness Brinell	Specific gravity
Mild steel	430	220	210	100–200	7.9
Low alloy steel	420–660	230–460	210	130–200	7.9
Cast iron	140–170	—	140	150–250	7.2
Stainless steel (18Cr, 8Ni)	>540	200	210	160	8.0
Nickel (>99 per cent Ni)	500	130	210	80–150	8.9
Monel	650	170	170	120–250	8.8
Copper (deoxidised)	200	60	110	30–100	8.9
Brass (Admiralty)	400–600	130	115	100–200	8.6
Aluminium (>99 per cent)	80–150	—	70	30	2.7
Dural	400	150	70	100	2.7
Lead	30	—	15	5	11.3
Titanium	500	350	110	150	4.5

Tensile strength

The tensile strength (tensile stress) is a measure of the basic strength of a material. It is the maximum stress that the material will withstand, measured by a standard tensile test.

Stiffness

Stiffness is the ability to resist bending and buckling.

Toughness

Toughness is associated with tensile strength, and is a measure of the material's resistance to crack propagation.

Hardness

The surface hardness, as measured in a standard test, is an indication of a material's ability to resist wear.

Fatigue

Fatigue failure is likely to occur in equipment subject to cyclic loading; for example, rotating equipment, such as pumps and compressors, and equipment subjected to pressure cycling.

Creep

Creep is the gradual extension of a material under a steady tensile stress, over a prolonged period of time. It is usually only important at high temperatures; for instance, with steam and gas turbine blades.

2. Effect of temperature on the mechanical properties

The tensile strength and elastic modulus of metals decrease with increasing temperature. For example, the tensile strength of mild steel (low carbon steel, C < 0.25 per cent) is 450 N/mm^2 at 25^{o}C falling to 210 at 500^{0}C, and the value of Young's modulus 200,000 N/mm^2 at 25^{o}C falling to 150,000 N/mm^2 at 500^{o}C. If equipment is being designed to operate at high temperatures, materials that retain their strength must be selected. Creep resistance will be important if the material is subjected to high stresses at elevated temperatures.

3. CORROSION RESISTANCE

The conditions that cause corrosion can arise in a variety of ways. For this brief discussion on the selection of materials it is convenient to classify corrosion into the following categories:

1. General wastage of material uniform corrosion.
2. Galvanic corrosion dissimilar metals in contact.
3. Pitting localized attack.
4. Intergranular corrosion.

Stress corrosion.

6. Erosion corrosion.
7. Corrosion fatigue.
8. High temperature oxidation.
9. Hydrogen embrittlement.

MATERIAL COSTS

An indication of the cost of some commonly used metals is given in Table 7.5. The actual cost of metals and alloys will fluctuate quite widely, depending on movements in the world metal exchanges. The quantity of a material used will depend on the material density and strength (design stress) and these must be taken into account when comparing material costs. cost rating factor defined by the equation:

$$\text{Cost rating} = \frac{C \times \rho}{\sigma_d} \tag{7.2}$$

where C = cost per unit mass, £/kg,
ρ = density, kg/m^3,
σ_d = design stress, N/mm^2.

Table 7.5. Basic cost of metals (mid-2004)

Metal	£/tonne	US$/US ton
Carbon steel	300	500
Low alloy steel (Cr-Mo)	400–500	700–850
Austenitic stainless steel		
304	1400	2400
316	1900	3200
Copper	1500	2500
Aluminium	900	1500
Aluminium alloy	850	1400
Nickel	6400	11,000
Monel	5000	8500
Titanium	20,000	34,000

Commonly Used Materials of Construction

The general mechanical properties, corrosion resistance, and typical areas of use of some of the materials commonly used in the construction of chemical plant are given in this section.

1. Iron and steel

Low carbon steel (mild steel) is the most commonly used engineering material. It is cheap; is available in a wide range of standard forms and sizes; and can be easily worked and welded. It has good tensile strength and ductility.

2. Stainless steel

The stainless steels are the most frequently used corrosion resistant materials in the chemical industry.

3. Nickel

Nickel has good mechanical properties and is easily worked. The pure metal (>99 per cent) is not generally used for chemical plant, its alloys being preferred for most applications. The main use is for equipment handling caustic alkalies at temperatures above that at which carbon steel could be used; above 70^0C. Nickel is not subject to corrosion cracking like stainless steel.

4. Monel

Monel, the classic nickel-copper alloy with the metals in the ratio 2 : 1, is probably, after the stainless steels, the most commonly used alloy for chemical plant. It is easily worked and has good mechanical properties up to 500ŽC. It is more expensive than stainless steel but is not susceptible to stress-corrosion cracking in chloride solutions. Monel has good resistance to dilute mineral acids and can be used in reducing conditions, where the stainless steels would be unsuitable. It may be used for equipment handling, alkalies, organic acids and salts, and sea water.

5. Copper and copper alloys

Pure copper is not widely used for chemical equipment. It has been used traditionally in the food industry, particularly in brewing. Copper is a relatively soft, very easily worked metal, and is used extensively for small-bore pipes and tubes. The main alloys of copper are the brasses, alloyed with zinc, and the bronzes, alloyed with tin. Other, so-called bronzes are the aluminium bronzes and the silicon bronzes. Copper is attacked by mineral acids, except cold, dilute, unaerated sulphuric acid.

6. Aluminum and its alloys

Pure aluminum lacks mechanical strength but has higher resistance to corrosion than its alloys.

Plastics as Materials of Construction for Chemical Plant

Plastics are being increasingly used as corrosion-resistant materials for chemical plant construction. Such as, Poly-vinyl chloride (PVC).

Rubber

Rubber, particularly in the form of linings for tanks and pipes, has been extensively used in the chemical industry for many years. Natural rubber is most commonly used, because of its good resistance to acids (except concentrated nitric) and alkalies. It is unsuitable for use with most organic solvents. Synthetic rubbers are also used for particular applications.

CHAPTER FIVE
DESIGN INFORMATION AND DATA

Information on manufacturing processes, equipment parameters, materials of construction, costs and the physical properties of process materials are needed at all stages of design; from the initial screening of possible processes, to the plant start-up and production. When a project is largely a repeat of a previous project, the data and information required for the design will be available in the Company's process files, if proper detailed records are kept. For a new project or process, the design data will have to be obtained from the literature, or by experiment (research laboratory and pilot plant), or purchased from other companies. The information on manufacturing processes available in the general literature can be of use in the initial stages of process design, for screening potential process; but is usually mainly descriptive, and too superficial to be of much use for detailed design and evaluation.

PREDICTION OF PHYSICAL PROPERTIES

1. DENSITY

1.1 Liquid density

Values for the density of pure liquids can usually be found in the handbooks. It should be noted that the density of most organic liquids, other than those containing a halogen or other "heavy atom", usually lies between 800 and 1000 kg/m^3.

$$\rho_b = \frac{M}{V_m} \tag{8.1}$$

where ρ_b = density, kg/m^3,
M = molecular mass,
V_m = molar volume, m^3/kmol.

Example 8.1

Calculate the density of a mixture of methanol and water at 20°C, composition 40 per cent w/w methanol.

Density of water at 20°C	998.2 kg/m^3
Density of methanol at 20°C	791.2 kg/m^3

Solution

Basis: 1000 kg

$$\text{Volume of water} = \frac{0.6 \times 1000}{998.2} = 0.601\ \text{m}^3$$

$$\text{Volume of methanol} = \frac{0.4 \times 1000}{791.2} = 0.506\ \text{m}^3$$

Total 1.107 m^3

$$\text{Density of mixture} = \frac{1000}{1.107} = \underline{\underline{903.3\ \text{kg/m}^3}}$$

Experimental value = 934.5 kg/m^3

$$\text{Error} = \frac{934.5 - 903.3}{903.3} = 3 \text{ per cent, which would be acceptable for most engineering purposes}$$

1.2 Gas and vapour density (specific volume)

For general engineering purposes it is often sufficient to consider that real gases, and vapours, behave ideally, and to use the gas law:

$$PV = n\mathrm{R}T \tag{8.3}$$

where P = absolute pressure $\mathrm{N/m^2}$ (Pa),
V = volume $\mathrm{m^3}$,
n = mols of gas
T = absolute temperature, K,
R = universal gas constant, 8.314 $\mathrm{J\ K^{-1}\ mol^{-1}}$ (or $\mathrm{kJ\ K^{-1}\ kmol^{-1}}$).

$$\text{Specific volume} = \frac{\mathrm{R}T}{P} \tag{8.4}$$

These equations will be sufficiently accurate up to moderate pressures, in circumstances where the value is not critical. If greater accuracy is needed, the simplest method is to modify equation 8.3 by including the compressibility factor z:

$$PV = zn\mathrm{R}T \tag{8.5}$$

2. VISCOSITY

Viscosity values will be needed for any design calculations involving the transport of fluids or heat.

2.1 Viscosity of Liquids

A rough estimate of the viscosity of a pure liquid at its boiling point can be obtained from the modified Arrhenius equation:

$$\mu_b = 0.01\rho_b^{0.5} \tag{8.8}$$

where μ_b = viscosity, $\mathrm{mNs/m^2}$,
ρ_b = density at boiling point, $\mathrm{kg/m^3}$.

A more accurate value can be obtained if reliable values of density are available, or can be estimated with sufficient accuracy, from Souders' equation, Souders (1938):

$$\log(\log 10\mu) = \frac{I}{M}\rho \times 10^{-3} - 2.9 \tag{8.9}$$

where μ = viscosity, $\mathrm{mNs/m^2}$,
M = molecular mass,
I = Souders' index, estimated from the group contributions given in Table 8.1,
ρ = density at the required temperature, $\mathrm{kg/m^3}$.

Example 8.2

Estimate the viscosity of toluene at 20°C.

Solution

Toluene

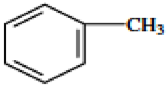
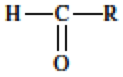
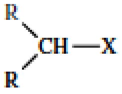
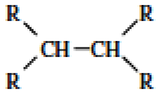
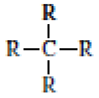


Table 8.1. Contributions for calculating the viscosity constant I in Souders' equation

Atom	H	O	C	N	Cl	Br	I
Contribution	+2.7	+29.7	+50.2	+37.0	+60	+79	+110

Contributions of groups and bonds

Double bond	−15.5	 $H-\underset{\underset{O}{\parallel}}{C}-R$	+10
Five-member ring	−24		
Six-member ring	−21		
Side groups on a six-member ring:		$-CH{=}CH-CH_2-X^{\dagger}$	+4
Molecular weight < 17	−9		+6
Molecular weight > 16	−17		
Ortho or *para* position	+3		
Meta position	−1		
	+8	OH	+57.1
		COO	+90
		COOH	+104.4
		NO_2	+80
	+10		
$-CH_2-$	+55.6		

† X is a negative group.

Contributions from Table 8.1:

7 carbon atoms	7×50.2	$= 351.4$
8 hydrogen atoms	8×2.7	$= 21.6$
3 double bonds	$3(-15.5)$	$= -46.5$
1 six-membered ring		-21.1
1 side group		-9.0
	Total, I	$= 296.4$

Density at 20°C = 866 kg/m^3
Molecular weight 92

$$\log(\log 10\mu) = \frac{296.4 \times 866 \times 10^{-3}}{92} - 2.9 = -0.11$$

$$\log 10\mu = 0.776$$

$$\mu = 0.597, \text{ rounded } = 0.6 \text{ mNs/m}^2$$

experimental value, 0.6 cp = 0.6 mNs/m^2

Variation with temperature

If the viscosity is known at a particular temperature, the value at another temperature can be estimated with reasonable accuracy by using the generalized plot Figure 8.1. The scale of the temperature ordinate is obtained by plotting the known value, as illustrated in Example 8.3.

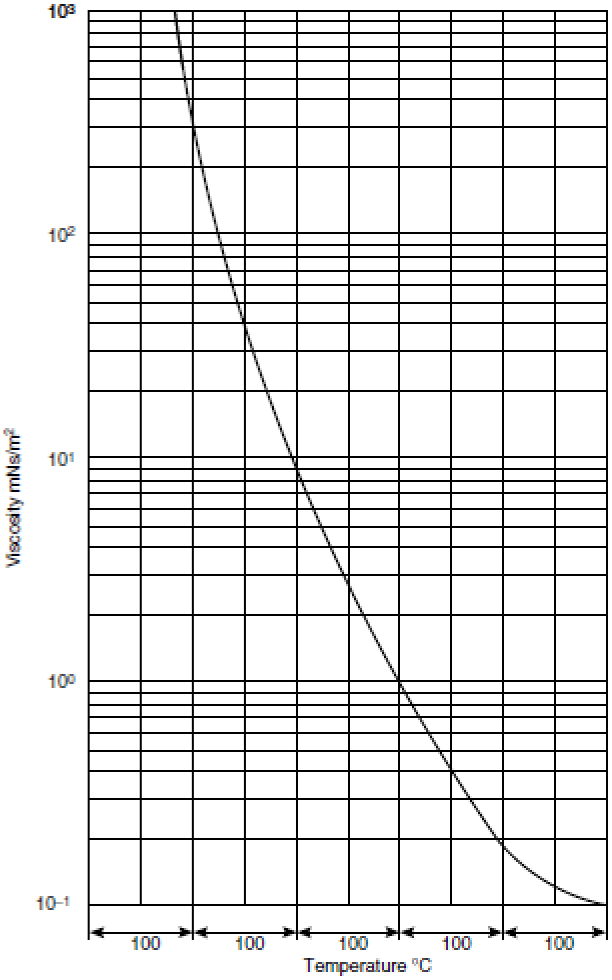


Figure 8.1. Generalised viscosity vs. temperature curve for liquids

Example 8.3

Estimate the viscosity of toluene at 80^{o}C, using the value at 20^{o}C given in Example 8.2.

Solution

Temperature increment 80 − 20 = 60°C.
From Figure 8.1*a*, viscosity at 80°C = 0.26 mN s/m^2.

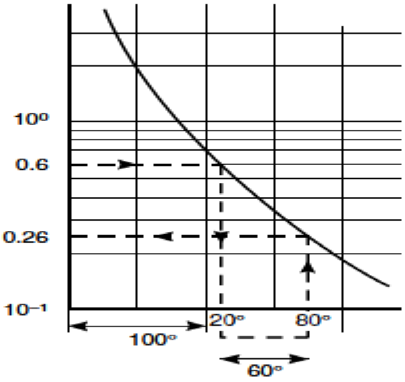


Figure 8.1*a*.

Effect of pressure

The viscosity of a liquid is dependent on pressure as well as temperature, but the effect is not significant except at very high pressures. A rise in pressure of 300 bar is roughly equivalent to a decrease in temperature of 1^{0}C.

Mixtures

It is difficult to predict the viscosity of mixtures of liquids. Viscosities are rarely additive, and the shape of the viscosity-concentration curve can be complex. The viscosity of the mixture may be lower or, occasionally, higher than that of the pure components. For a binary mixture equation 8.9 becomes:

$$\log(\log 10\ \mu_m) = \rho_m \left[\frac{x_1 I_1 + x_2 I_2}{x_1 M_1 + x_2 M_2}\right] \times 10^{-3} - 2.9 \qquad (8.10)$$

where μ_m = viscosity of mixture,
ρ_m = density of mixture,
x_1, x_2 = mol fraction of components,
M_1, M_2 = molecular masses of components.

For heat-transfer calculations

$$\frac{1}{\mu_m} = \frac{w_1}{\mu_1} + \frac{w_2}{\mu_2} \qquad (8.11)$$

where w_1, w_2 = mass fractions of the components 1 and 2,
μ_1, μ_2 = viscosities of components 1 and 2.

Gases

Reliable methods for the prediction of gas viscosities, and the effect of temperature and pressure. Where an estimate of the viscosity is needed to calculate Prandtl numbers (see Volume 1, Chapter 1) the methods developed for the direct estimation of Prandtl numbers should be used.

For gases at low pressure

	Prandtl number
Monatomic gases (e.g. Ar, He)	0.67 ± 5 per cent
Non-polar, linear molecules (e.g. O_2, Cl_2)	0.73 ± 15 per cent
Non-polar, non-linear molecules (e.g. CH_4, C_6H_6)	0.79 ± 15 per cent
Strongly polar molecules (e.g. CH_3OH, SO_2, HCl)	0.86 ± 8 per cent

The Prandtl number for gases varies only slightly with temperature.

THERMAL CONDUCTIVITY

The experimental methods used for the determination of thermal conductivity are described in books, which lists values for many substances.

Solids

The thermal conductivity of a solid is determined by its form and structure, as well as composition. Values for the commonly used engineering materials are given in various handbooks.

Liquids

The Weber equation can be used to make a rough estimate of the thermal conductivity of organic liquids, for use in heat-transfer calculations.

$$k = 3.56 \times 10^{-5} C_p \left(\frac{\rho^4}{M}\right)^{1/3} \qquad (8.12)$$

where k = thermal conductivity. W/m°C,
M = molecular mass,
C_p = specific heat capacity, kJ/kg°C,
ρ = density, kg/m^3.

Example

Estimate the thermal conductivity of benzene at 30°C.

Solution

Density at 30°C = 875 kg/m^3
Molecular mass = 78
Specific heat capacity = 1.75 kJ/kg°C

$$k = 3.56 \times 10^{-5} \times 1.75 \left(\frac{875^4}{78}\right)^{1/3} = \underline{\underline{0.12\ \text{W/m°C}}} \qquad (8.12)$$

Experimental value, 0.16 W/m°C

Gases

Approximate values for the thermal conductivity of pure gases, up to moderate pressures, can be estimated from values of the gas viscosity, using Eucken's equation:

$$k = \mu \left(C_p + \frac{10.4}{M} \right) \tag{8.13}$$

where
μ = viscosity, mNs/m^2, C_p = specific heat capacity, kJ/kg°C, M = molecular mass

Example

Estimate the thermal conductivity of ethane at 1 bar and 450^{0}C.

Solution

Viscosity = 0.0134 mNs/m^2
Specific heat capacity = 2.47 kJ/kg°C

$$k = 0.0134 \left(2.47 + \frac{10.4}{30} \right) = 0.038 \text{ W/m°C} \tag{8.13}$$

Experimental value, 0.043 W/m°C, error 12 per cent.

Mixtures

In general, the thermal conductivities of liquid mixtures, and gas mixtures, are not simple functions of composition and the thermal conductivity of the components. If the components are all non-polar a simple weighted average is usually sufficiently accurate for design purposes.

$$k_m = k_1 w_1 + k_2 w_2 + \cdots \tag{8.14}$$

where k_m = thermal conductivity of mixture,
k_1, k_2 = thermal conductivity of components,
w_1, w_2 = component mass fractions.

SPECIFIC HEAT CAPACITY

The specific heats of the most common organic and inorganic materials can usually be found in the handbooks.

Solids and liquids

Approximate values can be calculated for solids, and liquids, by using a modified form of Kopp's law. The heat capacity of a compound is taken as the sum of the heat capacities of the individual elements of which it is composed. The values attributed to each element, for liquids and solids, at room temperature, are given in Table 8.2; the method illustrated in Example 8.6.

Table 8.2. Heat capacities of the elements, J/mol°C

Element	Solids	Liquids
C	7.5	11.7
H	9.6	18.0
B	11.3	19.7
Si	15.9	24.3
O	16.7	25.1
F	20.9	29.3
P and S	22.6	31.0
all others	26.0	33.5

Example 8.6

Estimate the specific heat capacity of urea, CH_4N_2O.

Solution

Element	mol. mass	Heat capacity	
C	12	$7.5 =$	7.5
H	4	$4 \times 9.6 =$	38.4
N	28	$2 \times 26.0 =$	52.0
O	16	$16.7 =$	16.7
	60		114.6 J/mol°C

$$\text{Specific heat capacity} = \frac{114.6}{60} = \underline{\underline{1.91\ \ \text{J/g°C}}}\ \ (\text{kJ/kg°C})$$

Experimental value 1.34 kJ/kg°C.

Kopp’s rule does not take into account the arrangement of the atoms in the molecule, and, at best, gives only very approximate. For organic liquids, the group contribution method proposed by Chueh and Swanson will give accurate predictions. The contributions to be assigned to each molecular group are given in Table 8.3 and the method illustrated in Examples 8.7 and 8.8. The specific heats of liquid mixtures can be estimated, with sufficient accuracy for most technical calculations, by taking heat capacities of the components as additive. For dilute aqueous solutions it is usually sufficient to take the specific heat of the solution as that of water.

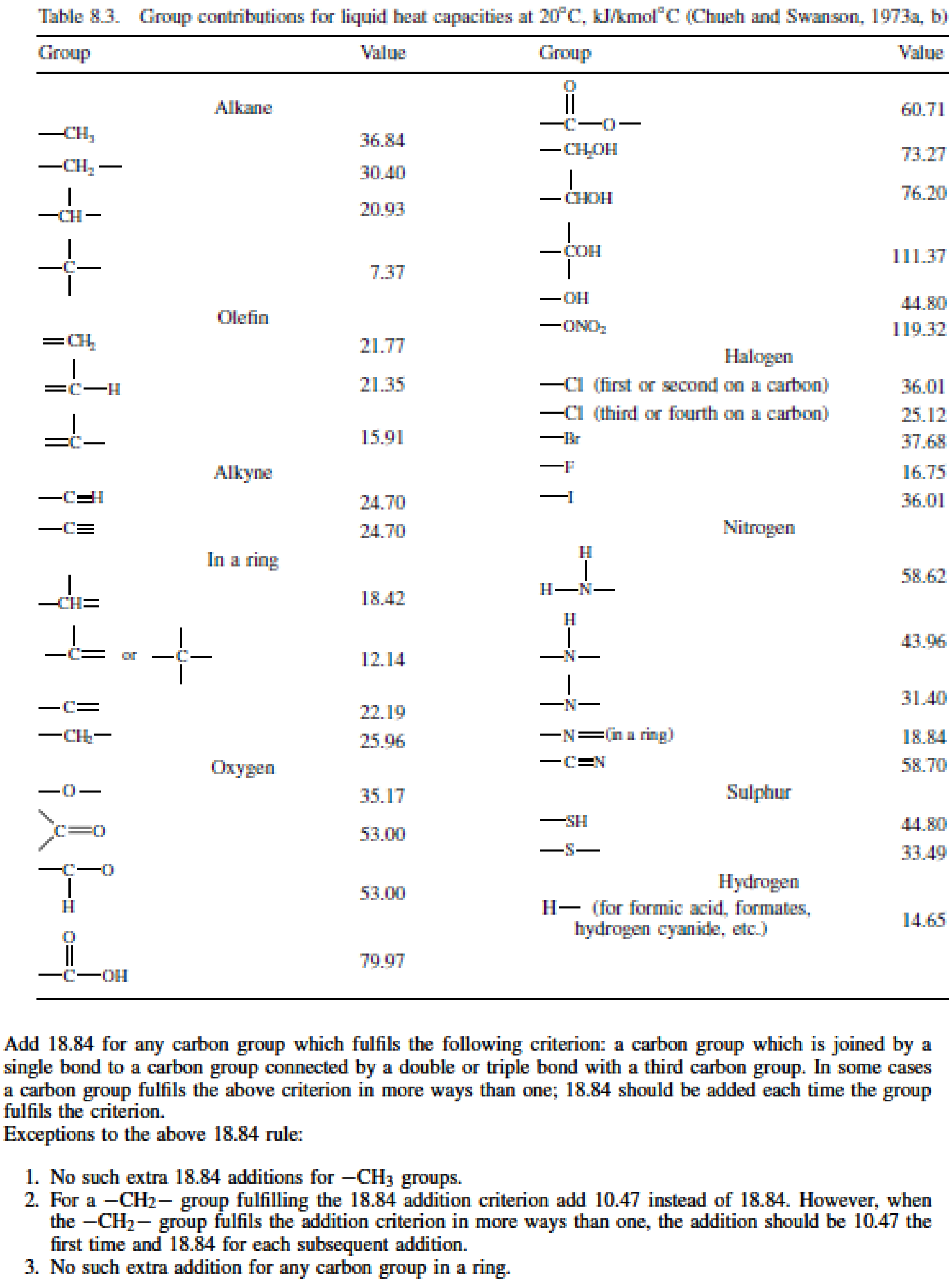


Table 8.3. Group contributions for liquid heat capacities at 20°C, kJ/kmol°C (Chueh and Swanson, 1973a, b)

Group	Value	Group	Value
Alkane		$-\overset{O}{\overset{\|}{C}}-O-$	60.71
$-CH_3$	36.84	$-CH_2OH$	73.27
$-CH_2-$	30.40	$-\overset{\|}{C}HOH$	76.20
$-\overset{\|}{C}H-$	20.93	$-\overset{\|}{\underset{\|}{C}}OH$	111.37
$-\overset{\|}{\underset{\|}{C}}-$	7.37	$-OH$	44.80
Olefin		$-ONO_2$	119.32
$=CH_2$	21.77	Halogen	
$=\overset{\|}{C}-H$	21.35	$-Cl$ (first or second on a carbon)	36.01
$=\overset{\|}{C}-$	15.91	$-Cl$ (third or fourth on a carbon)	25.12
Alkyne		$-Br$	37.68
$-C\equiv H$	24.70	$-F$	16.75
$-C\equiv$	24.70	$-I$	36.01
In a ring		Nitrogen	
$-\overset{\|}{C}H=$	18.42	$H-\overset{H}{\overset{\|}{N}}-$	58.62
$-\overset{\|}{C}=$ or $-\overset{\|}{\underset{\|}{C}}-$	12.14	$-\overset{H}{\overset{\|}{N}}-$	43.96
$-C=$	22.19	$-\overset{\|}{N}-$	31.40
$-CH_2-$	25.96	$-N=$ (in a ring)	18.84
Oxygen		$-C\equiv N$	58.70
$-O-$	35.17	Sulphur	
$\rangle C=O$	53.00	$-SH$	44.80
$-\underset{H}{\underset{\|}{C}}-O$	53.00	$-S-$	33.49
$-\overset{O}{\overset{\|}{C}}-OH$	79.97	Hydrogen	
		$H-$ (for formic acid, formates, hydrogen cyanide, etc.)	14.65

Add 18.84 for any carbon group which fulfils the following criterion: a carbon group which is joined by a single bond to a carbon group connected by a double or triple bond with a third carbon group. In some cases a carbon group fulfils the above criterion in more ways than one; 18.84 should be added each time the group fulfils the criterion.

Exceptions to the above 18.84 rule:

1. No such extra 18.84 additions for $-CH_3$ groups.
2. For a $-CH_2-$ group fulfilling the 18.84 addition criterion add 10.47 instead of 18.84. However, when the $-CH_2-$ group fulfils the addition criterion in more ways than one, the addition should be 10.47 the first time and 18.84 for each subsequent addition.
3. No such extra addition for any carbon group in a ring.

Example 8.7

Using Chueh and Swanson's method, estimate the specific heat capacity of ethyl bromide at 20°C.

Solution

Ethyl bromide CH_3CH_2Br

Group	Contribution	No. of		
$-CH_3$	36.84	1	=	36.84
$-CH_2-$	30.40	1	=	30.40
$-Br$	37.68	1	=	37.68
		Total		104.92 kJ/kmol°C

mol. wt. = 109

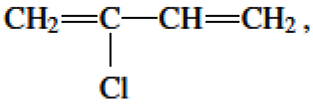
$$\text{Specific heat capacity} = \frac{104.92}{109} = \underline{\underline{0.96\ \text{kJ/kg°C}}}$$

Experimental value 0.90 kJ/kg°C

Example 8.8

Estimate the specific heat capacity of chlorobutadiene at 20°C, using Chueh and Swanson's method.

Solution

Structural formula 

$CH_2{=}\underset{\displaystyle Cl}{\underset{|}{C}}{-}CH{=}CH_2$, mol. wt. 88.5

Group	Contribution	No. of	Addition rule		Total
$=CH_2$	21.77	2	—	=	43.54
$=\underset{\vert}{C}-$	15.91	1	18.84	=	34.75
$=\overset{\vert}{CH}$	21.35	1	18.84	=	40.19
$-Cl$	36.01	1	—	=	36.01
					154.49 kJ/kmol°C

$$\text{Specific heat capacity} = \frac{154.49}{88.5} = \underline{\underline{1.75\ \text{kJ/kg°C}}}$$

Gases

The dependence of gas specific heats on temperature was discussed in Chapter 3, Section 3.5. For a gas in the ideal state the specific heat capacity at constant pressure is given by:

$$C_p^\circ = a + bT + cT^2 + dT^3 \qquad \text{(equation 3.19)}$$

Values for the constants in this equation for the more common gases can be found in the handbooks, and in Appendix C.

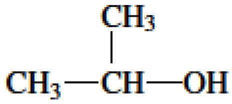
Several group contribution methods have been developed for the estimation of the constants, such as that by Rihani and Doraiswamy (1965) for organic compounds. Their values for each molecular group are given in Table 8.4, and the method illustrated in Example 8.9. The values should not be used for acetylenic compounds.

Example 8.9

Estimate the specific heat capacity of isopropyl alcohol at 500 K.

Solution

Structural formula



$$CH_3-\overset{\displaystyle CH_3}{\overset{|}{C}H}-OH$$

Group	No. of	a	$b \times 10^2$	$c \times 10^4$	$d \times 10^6$
$-CH_3$	2	5.0970	17.9480	−0.7134	0.0095
$-\overset{\vert}{\underset{\vert}{C}}H$	1	−14.7516	14.3020	−1.1791	0.03356
$-OH$	1	27.2691	−0.5640	0.1733	−0.0068
Total		17.6145	31.6860	−1.7190	0.0363

$$C_p^\circ = 17.6145 + 31.6860 \times 10^{-2}T - 1.7192 \times 10^{-4}T^2 + 0.0363 \times 10^{-6}T^3.$$

At 500 K, substitution gives:

$$C_p = \underline{\underline{137.6 \text{ kJ/kmol°C}}}$$

Experimental value, 31.78 cal/mol°C = 132.8 kJ/kmol°C, error 4 per cent.

ENTHALPY OF VAPORISATION (LATENT HEAT)

The latent heats of vaporisation of the more commonly used materials can be found in the handbooks and in Appendix C. A very rough estimate can be obtained from Trouton's rule (Trouton, 1884), one of the oldest prediction methods.

$$\frac{L_v}{T_b} = \text{constant} \tag{8.15}$$

where L_v = latent heat of vaporisation, kJ/kmol,
T_b = normal boiling point, K.

For organic liquids the constant can be taken as 100. More accurate estimates, suitable for most engineering purposes, can be made from knowledge of the vapour pressure-temperature relationship for the substance. Several correlations have been proposed and derived from the Antoine vapour pressure equation (see Section 8.11).

$$L_v = \frac{8.32\, BT^2 \Delta z}{(T + C)^2} \tag{8.16}$$

where L_v = latent heat at the required temperature, kJ/kmol,
T = temperature, K,
B, C = coefficients in the Antoine equation (equation 8.20),
$\Delta z = z_{\text{gas}} - z_{\text{liquid}}$ (where z is the compressibility constant), calculated from the equation:

$$\Delta z = \left[1 - \frac{P_r}{T_r^3}\right]^{0.5} \tag{8.17}$$

P_r = reduced pressure,
T_r = reduced temperature.

If an experimental value of the latent heat at the boiling point is known, the Watson equation (Watson, 1943), can be used to estimate the latent heat at other temperatures.

$$L_v = L_{v,b}\left[\frac{T_c - T}{T_c - T_b}\right]^{0.38} \tag{8.18}$$

where L_v = latent heat at temperature T, kJ/kmol,
$L_{v,b}$ = latent heat at the normal boiling point, kJ/kmol,
T_b = boiling point, K,
T_c = critical temperature, K,
T = temperature, K.

Mixtures

For design purposes it is usually sufficiently accurate to take the latent heats of the components of a mixture as additive:

$$L_v \text{ mixture } = L_{v1}x_1 + L_{v2}x_2 + \cdots \tag{8.19}$$

where L_{v1}, L_{v2} = latent heats of the components kJ/kmol,
x_1, x_2 = mol fractions of components.

Example 8.10

Estimate the latent heat of vaporisation of acetic anhydride, $C_4H_6O_3$, at its boiling point, 139.6°C (412.7 K), and at 200°C (473 K).

Solution

For acetic anhydride $T_c = 569.1$ K, $P_c = 46$ bar,

$$\text{Antoine constants } A = 16.3982$$
$$B = 3287.56$$
$$C = -75.11$$

Experimental value at the boiling point 41,242 kJ/kmol.

From Trouton's rule:

$$L_{v,b} = 100 \times 412.7 = \underline{\underline{41{,}270 \text{ kJ/kmol}}}$$

Note: the close approximation to the experimental value is fortuitous, the rule normally gives only a very approximate estimate.

From Haggenmacher's equation:

$$\text{at the b.p. } P_r = \frac{1}{46} = 0.02124$$

$$T_r = \frac{412.7}{569.1} = 0.7252$$

$$\Delta z = \left[1 - \frac{0.02124}{0.7252^3}\right]^{0.5} = 0.972$$

$$L_{v,b} = \frac{8.32 \times 3287.6 \times (412.7)^2 \times 0.972}{(412.7 - 75.11)^2} = \underline{\underline{39{,}733 \text{ kJ/mol}}}$$

At 200°C, the vapour pressure must first be estimated, from the Antoine equation:

$$\ln P = A - \frac{B}{T + C}$$

$$\ln P = 16.3982 - \frac{3287.56}{473 - 75.11} = 8.14$$

$$P = 3421.35 \text{ mmHg} = 4.5 \text{ bar}$$

$$P_c = \frac{4.5}{46} = 0.098$$

$$T_c = \frac{473}{569.1} = 0.831$$

$$\Delta z = \left[1 - \frac{0.098}{0.831^3}\right]^{0.5} = 0.911$$

$$L_v = \frac{8.32 \times 3287.6 \times (473)^2 \times 0.911}{(473 - 75.11)^2} = \underline{\underline{35{,}211 \text{ kJ/kmol}}}$$

Using Watson's equation and the experimental value at the b.p.

$$L_v = 41{,}242\left[\frac{569.1-473}{569.1-412.7}\right]^{0.38} = \underline{\underline{34{,}260\ \text{kJ/kmol}}}$$

VAPOUR PRESSURE

If the normal boiling point (vapour pressure = 1 atm) and the critical temperature and pressure are known, then a straight line drawn through these two points on a plot of log pressure versus reciprocal absolute temperature can be used to make a rough estimation of the vapour pressure at intermediate temperatures. Several equations have been developed to express vapour pressure as a function of temperature. One of the most commonly used is the three-term Antoine equation, Antoine (1888):

$$\ln P = A - \frac{B}{T+C} \tag{8.20}$$

where P = vapour pressure, mmHg,

A, B, C = the Antoine coefficients,

T = temperature, K.

DIFFUSION COEFFICIENTS (DIFFUSIVITIES)

Diffusion coefficients are needed in the design of mass transfer processes; such as gas absorption, distillation, and liquid-liquid extraction.

Gases

The equation developed by Fuller *et al.* (1966) is easy to apply and gives reliable estimates:

$$D_v = \frac{1.013\times10^{-7}T^{1.75}\left(\frac{1}{M_a}+\frac{1}{M_b}\right)^{1/2}}{P\left[\left(\sum_a v_i\right)^{1/3}+\left(\sum_b v_i\right)^{1/3}\right]^2} \tag{8.21}$$

where D_v = diffusivity, m^2/s,

T = temperature, K,

M_a, M_b = molecular masses of components a and b,

P = total pressure, bar,

$\sum_a v_i, \sum_b v_i$ = the summation of the special diffusion volume coefficients for components a and b, given in Table 8.5.

Table 8.5. Special atomic diffusion volumes (Fuller *et al.*, 1966)

Atomic and structural diffusion volume increments

C	16.5	Cl	19.5*
H	1.98	S	17.0*
O	5.48	Aromatic or hetrocyclic rings	−20.0
N	5.69*		

Diffusion volumes of simple molecules

H_2	7.07	CO	18.9
D_2	6.70	CO_2	26.9
He	2.88	N_2O	35.9
N_2	17.9	NH_3	14.9
O_2	16.6	H_2	12.7
Air	20.1	CCL_2F_2	114.8*
Ne	5.59	SF_6	69.7*
Ar	16.1	Cl_2	37.7*
Kr	22.8	Br_2	67.2*
Xe	37.9*	SO_2	41.1*

*Value based on only a few data points

Example 8.11

Estimate the diffusivity of methanol in air at atmospheric pressure and 25°C.

Solution

Diffusion volumes from Table 8.5; methanol:

Element	v_i		No. of		
C	16.50	×	1	=	16.50
H	1.98	×	4	=	7.92
O	5.48	×	1	=	5.48
			$\sum_a v_i$		29.90

Diffusion volume for air = 20.1.
1 standard atmosphere = 1.013 bar.
molecular mass CH_3OH = 32, air = 29.

$$D_v = \frac{1.013 \times 10^{-7} \times 298^{1.75}(1/32 + 1/29)^{1/2}}{1.013[(29.90)^{1/3} + (20.1)^{1/3}]^2} \qquad (8.21)$$

$$= \underline{\underline{16.2 \times 10^{-6} \mathrm{m}^2/\mathrm{s}}}$$

Experimental value, 15.9×10^{-6} m^2/s.

Liquids

The equation developed by Wilke and Chang (1955), given below, can be used to predict liquid diffusivity. This equation is discussed in Volume 1, Chapter 10.

$$D_L = \frac{1.173 \times 10^{-13}(\phi M)^{0.5} T}{\mu V_m^{0.6}} \tag{8.22}$$

where D_L = liquid diffusivity, m^2/s,
ϕ = an association factor for the solvent,
= 2.6 for water (some workers recommend 2.26),
= 1.9 for methanol,
= 1.5 for ethanol,
= 1.0 for unassociated solvents,
M = molecular mass of solvent,
μ = viscosity of solvent, $mN\ s/m^2$,
T = temperature, K,
V_m = molar volume of the solute at its boiling point, $m^3/kmol$. This can be estimated from the group contributions given in Table 8.6.

The method is illustrated in Example 8.12.

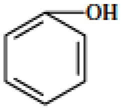
The Wilke-Chang correlation is shown graphically in Figure 8.2. This figure can be used to determine the association constant for a solvent from experimental values for D_L in the solvent.

The Wilke-Chang equation gives satisfactory predictions for the diffusivity of organic compounds in water but not for water in organic solvents.

Example 8.12

Estimate the diffusivity of phenol in ethanol at 20°C (293 K).

Solution

Viscosity of ethanol at 20°C, 1.2 mNs/m^2.
Molecular mass, 46.
Molar volume of phenol  from Table 8.6:

Atom	Vol.		No. of		
C	0.0148	×	6	=	0.0888
H	0.0037	×	6	=	0.0222
O	0.0074	×	1	=	0.0074
ring	−0.015	×	1	=	−0.015
					0.1034 $m^3/k\ mol$

$$D_L = \frac{1.173 \times 10^{-13}(1.5 \times 46)^{0.5} 293}{1.2 \times 0.1034^{0.6}} = \underline{\underline{9.28 \times 10^{-10}\ m^2/s}} \tag{8.22}$$

Experimental value, $8 \times 10^{-10}\ m^2/s$

Table 8.6. Structural contributions to molar volumes, m^3/kmol (Gambil, 1958)

Molecular volumes							
Air	0.0299	CO_2	0.0340	H_2S	0.0329	NO	0.0236
Br_2	0.0532	COS	0.0515	I_2	0.0715	N_2O	0.0364
Cl_2	0.0484	H_2	0.0143	N_2	0.0312	O_2	0.0256
CO	0.0307	H_2O	0.0189	NH_3	0.0258	SO_2	0.0448

Atomic volumes							
As	0.0305	F	0.0087	P	0.0270	Sn	0.0423
Bi	0.0480	Ge	0.0345	Pb	0.0480	Ti	0.0357
Br	0.0270	H	0.0037	S	0.0256	V	0.0320
C	0.0148	Hg	0.0190	Sb	0.0342	Zn	0.0204
Cr	0.0274	I	0.037	Si	0.0320		

Cl, terminal, as in RCl	0.0216	in higher esters, ethers	0.0110
medial, as in R—CHCl—R	0.0246	in acids	0.0120
Nitrogen, double-bonded	0.0156	in union with S, P, N	0.0083
triply bonded, as in nitriles	0.0162	three-membered ring	−0.0060
in primary amines, RNH_2	0.0105	four-membered ring	−0.0085
in secondary amines, R_2NH	0.012	five-membered ring	−0.0115
in tertiary amines, R_3N	0.0108	six-membered ring as in benzene, cyclohexane, pyridine	−0.0150
Oxygen, except as noted below	0.0074		
in methyl esters	0.0091	Naphthalene ring	−0.0300
in methyl ethers	0.0099	Anthracene ring	−0.0475

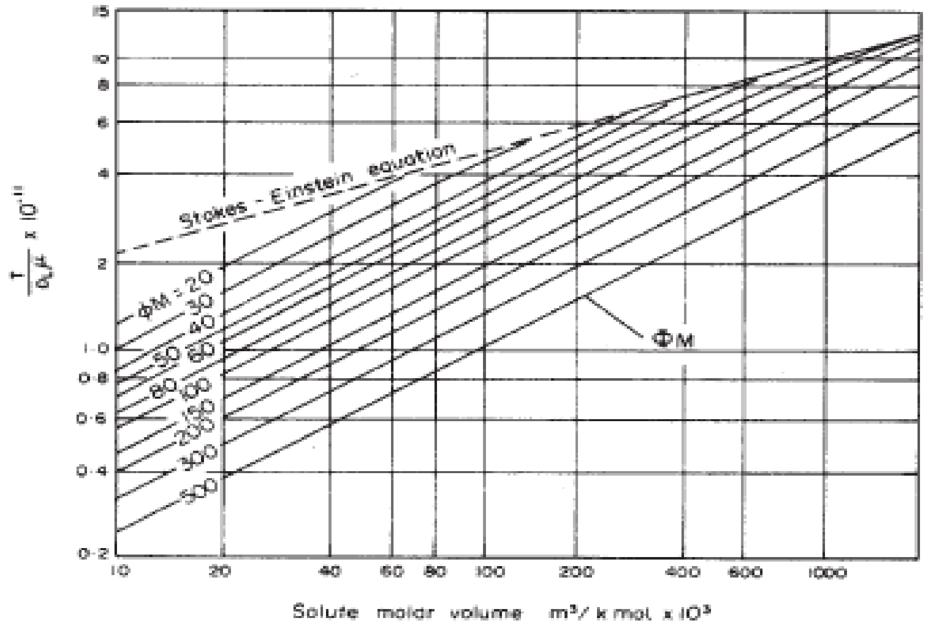


Figure 8.2. The Wilke-Chang correlation

Note: more details about other physical properties can be found in Chemical Engineering, Volume 6, Fourth edition, Chemical Engineering Design, R. K. Sinnott, Chapter 8.