

Design Information and Data

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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 startup and production.

Sources of Information on Manufacturing Processes

The chemical process industries are competitive, and the information that is published on commercial processes is restricted.

The articles on particular processes published in the technical literature and in textbooks invariably give only a superficial account of the chemistry and unit operations used.

They lack the detailed information on reaction kinetics, process conditions, equipment parameters, and physical properties that is needed for process design.

The **information** that can be found in the **general literature** is, however, useful in the **early stages** of a project.

The most **comprehensive** collection of information on manufacturing processes is **probably** the **Encyclopedia of Chemical Technology** edited by Kirk (2003) and Kirk and Othmer (2001), which covers the **whole range** of **chemical** and **associated products**.

The **extensive** German reference work on industrial processes, **Ullman's Encyclopedia of Industrial Technology**.

Patents

Patents can be useful **sources of information**, but some care is needed in **extracting information** from them.

To obtain a patent, an inventor is **legally obliged** to disclose the best mode of **practice** of the invention; **failure to do so** could render the patent invalid if it were **contested**.

Most patents therefore **include** one or more examples **illustrating** how the **invention is practiced** and differentiating it from the **prior art**.

When data from patents is used, it is **important** to carefully read the **section** that **describes** the experimental **procedure to be sure** that the experiments were run under **appropriate conditions**.

Patent attorneys generally try to write patents to claim **broad ranges** of **process conditions**.

So as to **maximize** the **range of validity** and make it hard for **competitors to avoid** the patent by making a slight change in temperature, pressure, or other process parameters.

The Internet

It is **worthwhile** searching online for **information** on **processes**, **equipment**, **products**, and **physical properties**.

Many manufacturers and government departments **maintain websites** and provide **up-to-date information** for the **health** and **environmental** effects of products.

Many university **libraries or engineering departments** provide information **guides for students**, and these are available on the Internet.

Some examples are

1. The University of Manchester, UK, Heriot-Watt University, Edinburgh, UK and the Joint Information Systems Committee: www.intute.ac.uk/sciences/
2. University of Florida Web Virtual Library: www.che.ufl.edu/www-che/
3. Karlsruhe University, Germany: International Directory of Chemical Engineering URLs: www.ciw.uni-karlsruhe.de/links.php

The American Chemical Society's Chemical Abstracts Service is the **best source** for **chemical properties** and **reaction kinetics** data.

General Sources of Physical Properties

International Critical Tables (1933) is still probably the most **comprehensive compilation** of **physical properties** and is available in most reference **libraries**.

physical properties **do not change**, except in as much as experimental techniques **improve**, and ICT is still a **useful** source of engineering data.

Tables and graphs of physical properties are given in many **handbooks** and **textbooks** on chemical engineering.

An **extensive compilation** of thermophysical data has been published by **Plenum Press** (Touloukian, 1970-1977). This **multiple-volume** work covers **conductivity**, **specific heat**, **thermal expansion**, **viscosity**, and **radiative properties** (emittance, reflectance, absorptance, and transmittance).

Elsevier have **published** a series of volumes on **physical property** and **thermodynamic data**.

The **Engineering Sciences Data Unit** (ESDU, www.ihsesdu.com) was set up to **provide validated data** for engineering design, **developed** under the **guidance** and **approval** of engineers from **industry**, the **universities**, and research **laboratories**.

ESDU data include equipment **design data** and **software** and extensive **high-quality** physical **property data**—mostly for **pure fluids** that are in use in the **oil** and **process** industries.

PPDS (**Physical Property Data Service**) was originally developed in the United Kingdom by the Institution of Chemical Engineers and the National Physical Laboratory.

The **DIPPR™** databases were developed in the United States by the Design Institute for Physical Properties of the American Institute of Chemical Engineers.

The DIPPR™ projects are **aimed** at providing **evaluated** process design data for the design of **chemical processes** and **equipment**.

Prediction of Physical Properties

Density

- Liquids

The density of most **organic liquids**, other than those **containing a halogen** or other "**heavy atom**," usually lies between 800 and 1000 kg/m³.

An **approximate estimate** of the density at the **normal boiling point** can be obtained from the molar volume

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

where

ρ_b = density, kg/m³;

M = molecular mass;

V_m = molar volume, m³/kmol.

If data on the **variation of density** with **temperature** cannot be found, they can be approximated for nonpolar liquids from **Smith's equation** for thermal expansion

(Smith et al., 1954):

$$\beta = \frac{0.04314}{(T_c - T)^{0.641}}$$

Where

β = coefficient of thermal expansion, K⁻¹;

T_c = critical temperature, K;

T = temperature, K.

- Gas and Vapor Density (Specific Volume)

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

$$PV = nRT$$

$$\text{Specific volume} = RT/P$$

These equations will be **sufficiently accurate** up to **moderate pressures**.

If greater **accuracy** is needed, the simplest method is to **modify** equation by including the **compressibility factor z**:

$$PV = znRT$$

The compressibility factor can be **estimated** from a **generalized compressibility plot**, which gives **z** as a **function** of reduced pressure and temperature

The **pseudocritical** properties of **mixtures** should be used to obtain the compressibility factor:

$$P_{c,m} = P_{c,a} \gamma_a + P_{c,b} \gamma_b + \dots$$

$$T_{c,m} = T_{c,a} \gamma_a + T_{c,b} \gamma_b + \dots$$

Viscosity

- **Liquids**

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

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

where

μ_b = viscosity, mNs/m²;

ρ_b = density at boiling point, kg/m³.

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

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

where

μ = viscosity, mNs/m²;

M = molecular mass;

I = Souders' index, estimated from the group contributions

ρ = density at the required temperature, kg/m³.

- **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.

As an **approximation**, a **weighted average** viscosity is calculated, if the **range** of viscosity is **not very wide**.

For a binary mixture,

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

For heat transfer calculations, Kern (1950) gives a **rough rule of thumb** for organic liquid mixtures:

$$\frac{1}{\mu_m} = \frac{w_1}{\mu_1} + \frac{w_2}{\mu_2}$$

where

w_1, w_2 = mass fractions of the components 1 and 2;

- **Gases**

Reliable methods for the prediction of gas viscosities and the **effect of temperature** and **pressure** are given by **Bretsznajder (1971)** and **Reid et al. (1987)**.

Where an **estimate of the viscosity** is needed to calculate Prandtl numbers, the methods developed for the **direct estimation of Prandtl numbers** should be used.

For gases at low pressure, **Bromley (1952)** has suggested the following values:

	Prandtl Number
Monatomic gases (e.g., Ar, He)	$0.67 \pm 5\%$
Nonpolar, linear molecules (e.g., O ₂ , Cl ₂)	$0.73 \pm 15\%$
Nonpolar, nonlinear molecules (e.g., CH ₄ , C ₆ H ₆)	$0.79 \pm 15\%$
Strongly polar molecules (e.g., CH ₃ OH, SO ₂ , HCl)	$0.86 \pm 8\%$

Thermal Conductivity

The experimental methods used for the **determination of thermal conductivity** are described by **Tsederberg** (1965). The **four volume handbook** by Yaws (1995-1997) is a useful source of thermal conductivity data for **hydrocarbons** and **inorganic** compounds.

- **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** (Weber, 1880) can be used to make a **rough estimate** of the thermal conductivity of organic liquids for use in heat transfer calculations:

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

where

k = thermal conductivity, W/m °C;

M = molecular mass;

C_p = specific heat capacity, kJ/kg °C;

ρ = density, kg/m³.

- **Gases**

The thermal conductivity of **pure gases**, up to **moderate pressures**, can be estimated from values of the **gas viscosity**, using **Eucken's equation** (Eucken, 1912):

$$k = \mu \left(c_p + \frac{10.4}{M} \right)$$

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.

Bretsznajder (1971) discusses the methods that are available for estimating the thermal conductivities of **mixtures** from a **knowledge** of the thermal conductivity of the components.

If the components are all **nonpolar**, a simple **weighted average** is usually sufficiently accurate for design purposes:

$$k_m = k_1 w_1 + k_2 w_2 + \dots \quad w_1, w_2 = \text{component mass fractions}$$

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**, which is given by **Werner** (1941).

The heat capacity of a **compound** is taken as the **sum of the heat capacities** of the **individual elements** of which it is composed.

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

Heat Capacities of the Elements, J/mol °C

Kopp's rule does not take into **account** the **arrangement of the atoms** in the **molecule** and, at best, gives only very **approximate**, "ballpark" values.

For organic liquids, the **group contribution** method proposed by **Chueh and Swanson** (1973a, b) gives reasonably **accurate predictions**.

Liquid specific heats do **not vary** much with **temperature**, at temperatures well below the critical temperature (reduced temperature < 0.7).

The specific heats of **liquid mixtures** can be estimated, with **sufficient accuracy** by taking heat capacities as the **mass (or mole) weighted sum** of the **pure component** heat capacities.

For **dilute aqueous solutions**, it is usually sufficient to take the **specific heat** of the solution as that of **water**.

- **Gases**

For a gas in the **ideal state** the specific heat capacity at **constant pressure** is given by

$$C_p = a + bT + cT^2 + dT^3$$

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

Several **group contribution methods** have been developed for the estimation of the constants, such as that by **Rihani and Doraiswamy** (1965) for organic compounds.

Enthalpy of Vaporization (Latent Heat)

A very **rough estimate** can be obtained from **Trouton's rule** (**Trouton, 1884**), one of the oldest prediction methods:

$$\frac{L_v}{T_b} = \text{constant} \quad \text{where}$$

L_v = latent heat of vaporization, 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 vapor pressure-temperature relationship for the substance.

The equation presented here, due to **Haggenmacher** (1946), is derived from the **Antoine vapor pressure equation**:

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

where

L_v = latent heat at the required temperature, kJ/kmol;

T = temperature, K;

B, C = coefficients in the Antoine equation

$\Delta z = z_{\text{gas}} - z_{\text{liquid}}$ (where z is the **compressibility constant**), calculated from the equation:

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

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**:

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

where

$L_{v,b}$ = latent heat at the **normal boiling point**, kJ/kmol.

Over a **limited range** of temperature, **up to 100°C**, the **variation** of latent heat with temperature can usually be taken as **linear**.

- **Mixtures**

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

$$L_v \text{ mixture} = L_{v1}x_1 + L_{v2}x_2 + \dots$$

Vapor Pressure

If the **normal boiling point** (vapor 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 **vapor pressure** at intermediate temperatures.

Several equations have been developed to **express vapor pressure** as a function of **temperature**. One of the **most commonly** used is the three-term **Antoine equation** (Antoine, 1888):

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

Diffusion Coefficients (Diffusivities)

Diffusion coefficients are **needed** in the design of **mass transfer processes**, such as **gas absorption**, **distillation**, and **liquid-liquid extraction**, as well as in **catalytic reactions** where mass transfer can **limit the rate of reaction**.

Experimental values for the **more common systems** can be often found in the **literature**, but for most design work the values must be estimated.

- **Gases**

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

$$D_v = \frac{1.013 \times 10^{-7} T^{1.75} \left(\frac{1}{M_a} + \frac{1}{M_b} \right)^{1/2}}{P [(\sum_d v_i)^{1/3} + (\sum_b v_i)^{1/3}]^2}$$

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.

- **Liquids**

The equation developed by **Wilke and Chang (1955)** can be used to predict **liquid diffusivity**:

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

where

D_L = liquid diffusivity, m²/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/m²;

T = temperature, K;

V_m = molar volume of the solute at its boiling point, m³/kmol. This can be estimated from the group contributions given in Table.

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

Surface Tension

It is usually difficult to find experimental values for surface tension for any but the more commonly used liquids.

A useful compilation of experimental values is that by Jasper (1972), which covers over 2000 pure liquids. Othmer et al. (1968) give a nomograph covering about 100 compounds.

If reliable values of the liquid and vapor density are available, the surface tension can be estimated from the Sugden parachor, which can be estimated by a group contribution method (Sugden, 1924):

$$\sigma = \left[\frac{P_{ch}(\rho_L - \rho_v)}{M} \right]^4 \times 10^{-12}$$

where

σ = surface tension, mJ/m² (dyne/cm);

P_{ch} = Sugden's parachor;

ρ_L = liquid density, kg/m³;

ρ_v = density of the saturated vapor, kg/m³;

M = molecular mass;

σ , ρ_L , ρ_v evaluated at the system temperature.

The vapor density can be neglected when it is small compared with the liquid density.

- **Mixtures**

The surface tension of a mixture is **rarely a simple function of composition**. However, for hydrocarbons a **rough value** can be calculated by assuming a **linear relationship**:

$$\sigma_m = \sigma_1 x_1 + \sigma_2 x_2 \dots$$

where
 σ_m = surface tension of mixture;
 σ_1, σ_2 = surface tension of components;
 x_1, x_2 = component mol fractions.

Critical Constants

Values of the **critical temperature** and **pressure** are needed for prediction methods that correlate **physical properties** with the **reduced conditions**.

It is also important to know the **critical conditions** when applying **equation of state methods**, as some of the equation of state models are **unreliable close to the critical point**.

Experimental values for **many substances** can be found in various **handbooks** and in **Appendix**. If **reliable experimental values** cannot be found, **techniques** are available for estimating the critical constants with **sufficient accuracy** for most design purposes.

For organic compounds, **Lydersen's method** is normally used (Lydersen, 1955):

$$T_c = \frac{T_b}{[0.567 + \sum \Delta T - (\sum \Delta T)^2]}$$

$$P_c = \frac{M}{[0.34 + \sum \Delta P]^2}$$

$$V_c = 0.04 + \sum \Delta V$$

where

T_c = critical temperature, K;

P_c = critical pressure, atm (1.0133 bar);

V_c = molar volume at the critical conditions, m³/kmol;

T_b = normal boiling point, K;

M = relative molecular mass;

ΔT = critical temperature increments,

ΔP = critical pressure increments,

ΔV = molar volume increments,

Phase Equilibrium Data

Phase equilibrium data are needed for the design of all separation processes that depend on differences in concentration between phases.

Experimental data have been published for several thousand binary and many multicomponent systems. All published data are comprised in volumes to DECHEMA, vapor-liquid and liquid-liquid data collection (DECHEMA, 1977).

- Phase Equilibrium

The thermodynamic equilibrium between two phases of a multicomponent mixture is that for every component, i

$$f_i^v = f_i^L$$

where f_i^v is the vapor-phase fugacity and f_i^L is the liquid-phase fugacity of component i :

$$f_i^v = P\phi_i y_i$$

and

$$f_i^L = f_i^{OL} \gamma_i x_i$$

where

P = total system pressure;

ϕ_i = vapor fugacity coefficient;

y_i = concentration of component i in the vapor phase;

f_i^{OL} = standard state fugacity of the pure liquid;

γ_i = liquid-phase activity coefficient;

x_i = concentration of component i in the liquid phase;

Substitution and rearrangement gives following relation

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i f_i^{OL}}{P \phi_i}$$

where

K_i is the distribution coefficient (the K value);

ϕ_i can be calculated from an appropriate equation of state;

f_i^{OL} can be **computed** from the following expression:

$$f_i^{OL} = P_i^o \phi_i^s \left\{ \exp \left\{ \frac{(P - P_i^o)}{RT} v_i^L \right\} \right\}$$

where

P_i^o = the pure component vapor pressure (which can be calculated from the Antoine equation; N/m²;

ϕ_i^s = the fugacity coefficient of the pure component i at saturation;

v_i^L = the liquid molar volume, m³/mol.

The **exponential term** in equation is known as the **Poynting correction** and corrects the **effects of pressure** on the **liquid-phase fugacity**.

ϕ_i^S is calculated using the same **equation of state** used to calculate ϕ_i .

For systems in which the **vapor phase imperfections** are not significant, equation reduces to the familiar **Raoult's law equation**:

$$K_i = \frac{\gamma_i P_i^0}{P}$$

- **Relative Volatility**

The **relative volatility of two components** can be expressed as the **ratio of their K values**:

$$\alpha_{ij} = \frac{K_i}{K_j}$$

For ideal mixtures (obeying Raoult's law):

$$K_i = \frac{P_i^0}{P} \quad \text{and}$$
$$\alpha_{ij} = \frac{K_i^0}{K_j^0} = \frac{P_i^0}{P_j^0}$$

where K_i^0 and K_j^0 are the ideal K values for components i and j.

- **K-values for Hydrocarbons**

A useful source of K-values for light hydrocarbons is the well-known "De Priester charts" (Dabyburjor, 1978).

These charts give the K-values over a wide range of temperature and pressure.

[Coulson & Richardson's Chemical Engineering. Vol. 6, Chemical Engineering Design.pdf](#)



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