



جامعة الملك فهد للبترول والمعادن
King Fahd University of Petroleum & Minerals

Introduction to Chemical Engineering

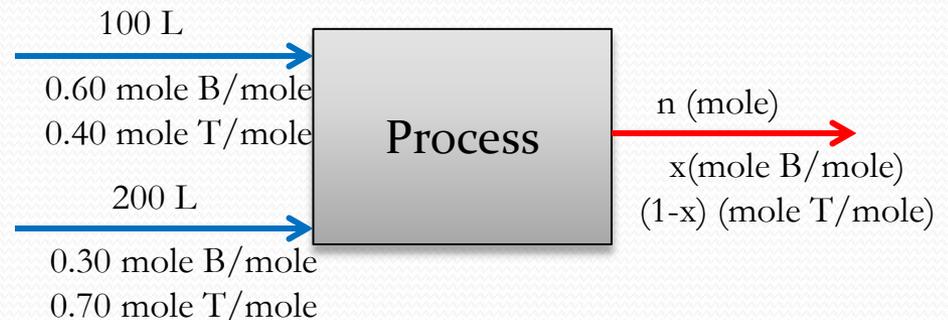
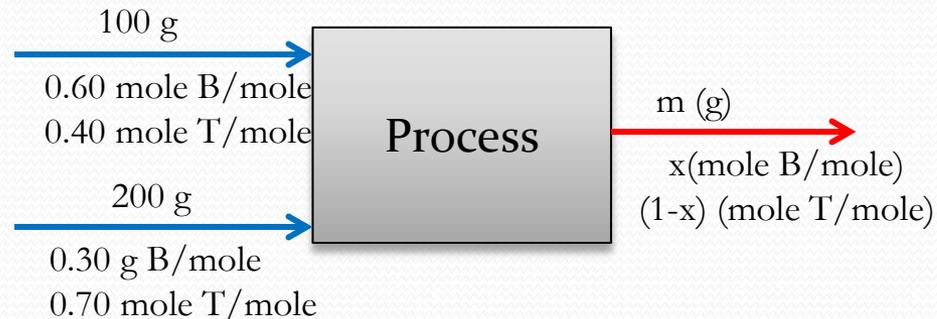
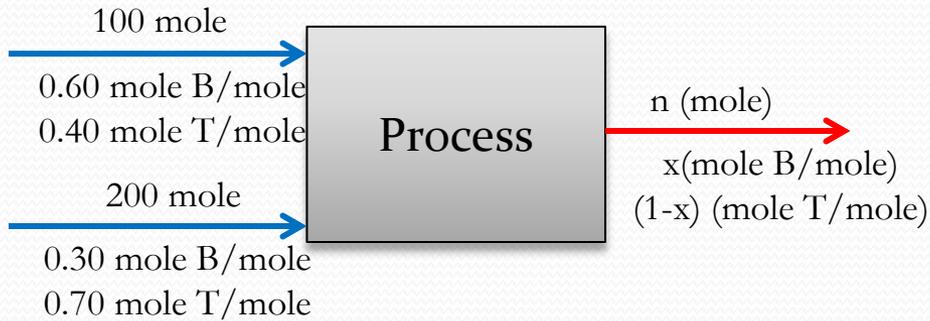
CHE-201

INSTRUCTOR: Dr. Nabeel Salim Abo-Ghander

Chapter 5

Single-Phase Systems

Introduction:



5.1 Liquids and Solid Densities:

Density of a substance is defined as the ratio of the mass of the substance to its volume.

Specific volume is the volume of a unit mass

$$\hat{V} = \frac{1}{\rho}$$

Density is denoted mathematically with the Greek symbol ρ

$$\rho = f(T, P)$$

For solid and liquids, density is independent of pressure and changes relatively small with temperature. **Densities of liquids and solids are assumed to be constant (incompressible)**

For Gases, density is a strong function of pressure and temperature. **Effects of temperature and pressure on gaseous systems can't be ignored.**

5.1 Liquids and Solid Densities:

For a mixture of n liquids, the density can be estimated by assuming:

1. Volume additivity:

$$\frac{1}{\bar{\rho}} = \sum_{i=1}^n \frac{x_i}{\rho_i}$$

2. Average the pure component densities, weighting each by one by the mass fraction of the component:

$$\bar{\rho} = \sum_{i=1}^n x_i \rho_i$$

Example 5.1-1: Determination of a Solution Density

Determine the density in g/cm^3 of a 50% aqueous solution of H_2SO_4 at 20°C , both by:

1. Looking up a tabulated value.
2. Assuming volume additivity of the solution components.

5.2 Ideal Gases:

Equation of State:

Equation relates the molar quantity and volume of a gas to temperature and pressure of the system.

Ideal Gas Equation of State:

$$PV = nRT \qquad P\hat{V} = RT$$

P: absolute pressure of a gas.

V (\dot{V}): volume (volumetric flowrate) of the gas.

n (\dot{n}): number of moles (molar flowrate) of the gas.

R: the gas constant, whose value depends on the units of P, V, n, and T.

T: absolute temperature of the gas.

5.2 Ideal Gases:

Values of the gas constant:

$$\begin{aligned}R &= 8.314 \text{ m}^3 \times \text{Pa} / (\text{mol} \times \text{K}) \\ &= 0.08314 \text{ L} \times \text{bar} / (\text{mol} \times \text{K}) \\ &= 62.36 \text{ L} \times \text{mmHg} / (\text{mol} \times \text{K}) \\ &= 0.7302 \text{ ft}^3 \times \text{atm} / (\text{lb} - \text{mol} \times {}^\circ\text{R}) \\ &= 8.314 \text{ J} / (\text{mol} \times \text{K})\end{aligned}$$

5.2 Ideal Gases:

Comments on an ideal gas law:

- ✓ It is an approximation, works for temperature above 0°C and pressure below 1.0 atm.
- ✓ This approximation can be measured by checking:

$$\varepsilon = \frac{X_{ideal} - X_{true}}{X_{true}} \times 100\%$$

$$|\varepsilon| < 1\% \quad \text{if} \quad \hat{V}_{ideal} = \frac{RT}{P} > 5\text{L/mol} \left(80\text{ft}^3/\text{lb-mole} \right) \quad (\text{diatomic gases})$$

$$> 20\text{L/mol} \left(320\text{ft}^3/\text{lb-mole} \right) \quad (\text{other gases})$$

- ✓ 1 mole of an ideal gas at 0°C and 1 atm pressure occupies 22.415 liters.

5.2 Ideal Gases:

Example 5.2-1: The Ideal Gas Equation of State

One hundred grams of nitrogen is stored in a container at 23.0°C and 3.00 psig.

1. Assuming ideal gas behavior, calculate the container volume in liters.
2. Verify that the ideal gas equation of state is a good approximation for the given conditions.

5.2 Ideal Gases:

To find the density of a gas using ideal gas law, we introduce:

$$\hat{V}\left(\frac{\text{liters}}{\text{mol}}\right) = \frac{\bar{M}(\text{g/mol})}{\rho(\text{g/liter})}$$

$$\rho = \frac{P\bar{M}}{RT}$$

5.2 Ideal Gases:



Is there a way to avoid using the values of the gas constant?

5.2 Ideal Gases:

Ideal gas law gives:

$$PV = nRT$$

Ideal gas law at standard conditions:

$$P_s \hat{V}_s = RT_s$$

Divide both equations:

$$\left(\frac{P}{P_s}\right)\left(\frac{V}{\hat{V}_s}\right) = n\left(\frac{T}{T_s}\right)$$

✓ Standard conditions are:

$$\text{Pressure} = 1.0 \text{ atm}$$

$$\text{Temperature} = 0^\circ\text{C}$$

✓ Volumes of any gas at these conditions are:

$$V_s = 22.4 \text{ m}^3(\text{STP})/\text{kmol} = 22.4 \text{ L}(\text{STP})/\text{mol} = 359 \text{ ft}^3 (\text{STP})/\text{lb-mole}$$

5.2 Ideal Gases:

Notations:

- ✓ Standard cubic meters (SCM) stands for $\text{m}^3(\text{STP})$.
- ✓ Standard cubic feet (SCF) stands for $\text{ft}^3(\text{STP})$.

Example: 18.2 SCMH means $18.2 \text{ m}^3/\text{h}$ at 0°C and 1 atm.

Question:

Can we have a gas flowrate given as: 23.8 SCMH at 150°C and 2.5 atm?

5.2 Ideal Gases:

Example 5.2-2: Conversion from Standard Conditions

Butane (C_4H_{10}) at $360^\circ C$ and 3.00 atm absolute flows into a reactor at a rate of 1100 kg/h. calculate the volumetric flow rate of this stream using conversion from standard conditions

5.2 Ideal Gases:

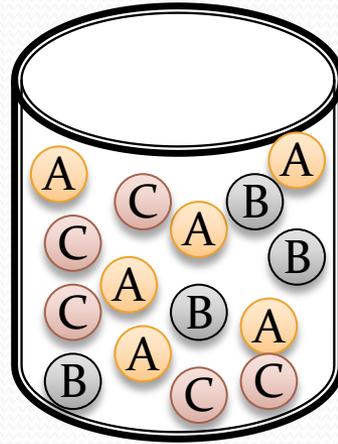
Example 5.2-3: Effect of T and P on Volumetric Flow Rates

Ten cubic feet of air at 70°F and 1.00 atm is heated to 610°F and compressed to 2.50 atm. What volume does the gas occupy in its final state?

Example 5.2-4: Standard and True Volumetric Flow Rates:

The flow rate of a methane stream at 285°F and 1.30 atm is measured with an orifice meter. The calibration chart for the meter indicates that the flow rate is 3.95×10^5 SCFH. Calculate the molar flowrate and the true volumetric flowrate of the stream.

5.2c Ideal Gas Mixtures:



$$PV = nRT$$

- ✓ Partial pressure of a component A is the pressure which would be exerted by the component alone at the same total volume V and the same temperature.

$$p_A V = n_A RT$$

$$\frac{p_A}{P} = \frac{n_A}{n} = y_A$$

$$p_A = y_A P$$

5.2c Ideal Gas Mixtures:

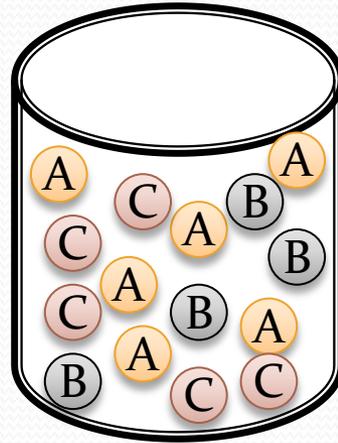
- ✓ The partial pressure of a component in an ideal gas mixture is the fraction of that component times the total pressure.

Dalton's law

The partial pressures of a components of an ideal gas mixture add up to the total pressure.

$$p_A + p_B + \dots = (y_A + y_B + \dots)P = P$$

5.2c Ideal Gas Mixtures:



$$PV = nRT$$

✓ Pure-component volume is the volume that would be occupied by n_A moles of A alone at the total pressure P and temperature T of the mixture.

$$Pv_A = n_A RT$$

$$\frac{v_A}{V} = \frac{n_A}{n} = y_A$$

$$v_A = y_A V$$

✓ Amagat's law: $v_A + v_B + \dots = (y_A + y_B + \dots)V = V$

5.2c Ideal Gas Mixtures:

Note:

- ✓ The quantity v_A/V is the volume fraction of A in the mixture.
- ✓ The volume fraction of a substance in an ideal gas mixture equals the mole fraction of this substance.

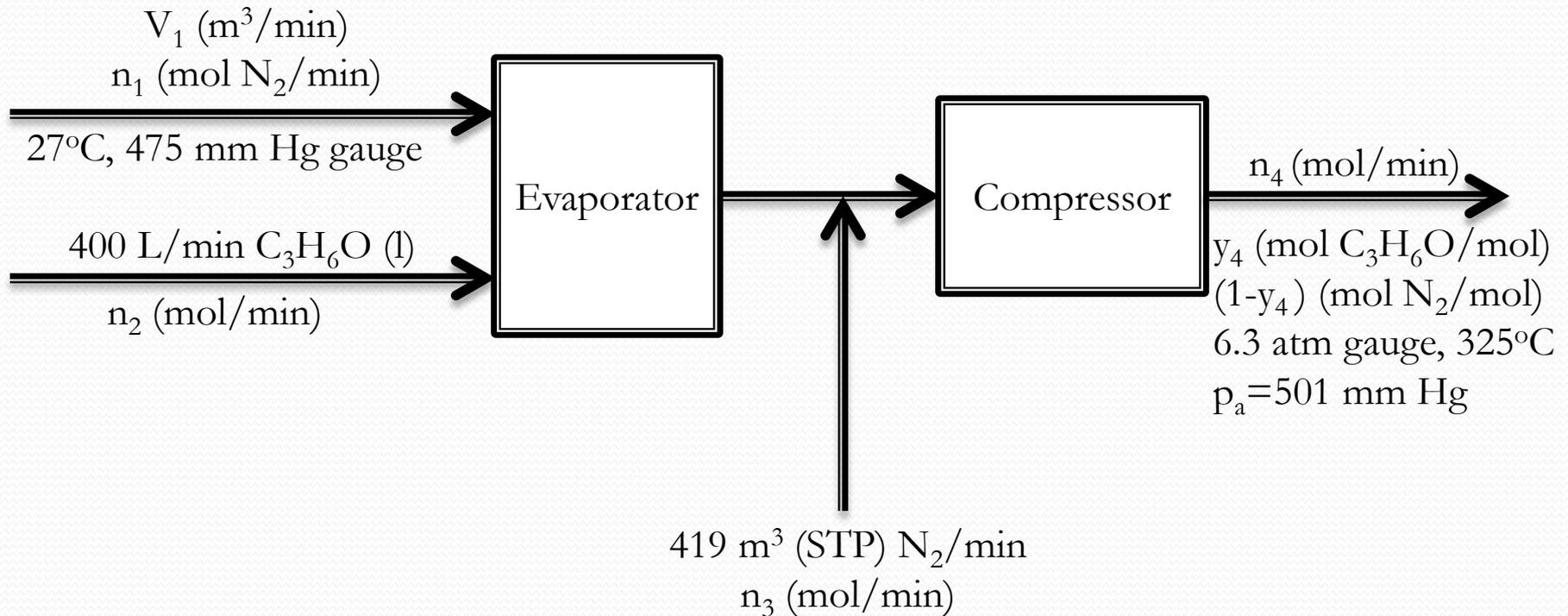
5.2c Ideal Gas Mixtures:

Example 5.2-5 Material Balances on an Evaporator-Compressor:

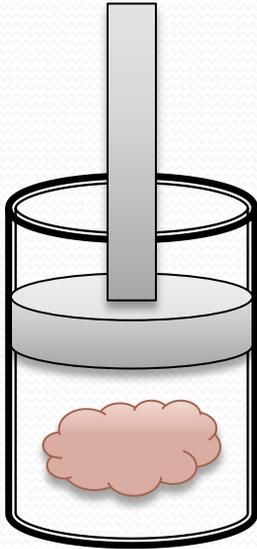
Liquid acetone ($\text{C}_3\text{H}_6\text{O}$) is fed at rate of 400 L/min into a heated chamber, where it evaporates into a nitrogen stream. The gas leaving the heater is diluted with another nitrogen stream flowing at a measured rate of 419 m^3 (STP)/min. The combined gases are then compressed to a total pressure $P = 6.3$ atm gauge at a temperature of 325°C . The partial pressure of acetone in this stream is $p_a = 501$ mm Hg. Atmospheric pressure is 763 mm Hg.

1. What is the molar composition of the stream leaving the compressor?
2. What is the volumetric flow rate of the nitrogen entering the evaporator if the temperature and pressure of this stream are 27°C and 475 mm Hg gauge?

5.2c Ideal Gas Mixtures:

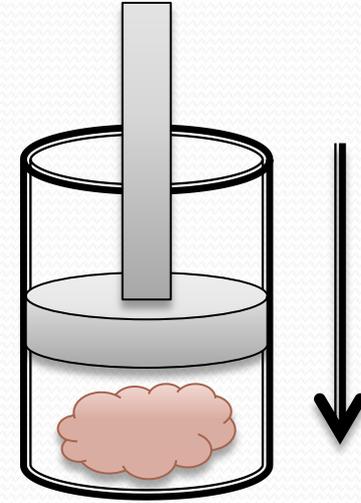


5.3 Equations of State for Nonideal Gases:



Temperature = 25 °C

$$P_{\text{cond}} = 0.0234$$
$$\rho_v = 0.0234 \text{ kg/m}^3$$
$$\rho_l = 997.0 \text{ kg/m}^3$$



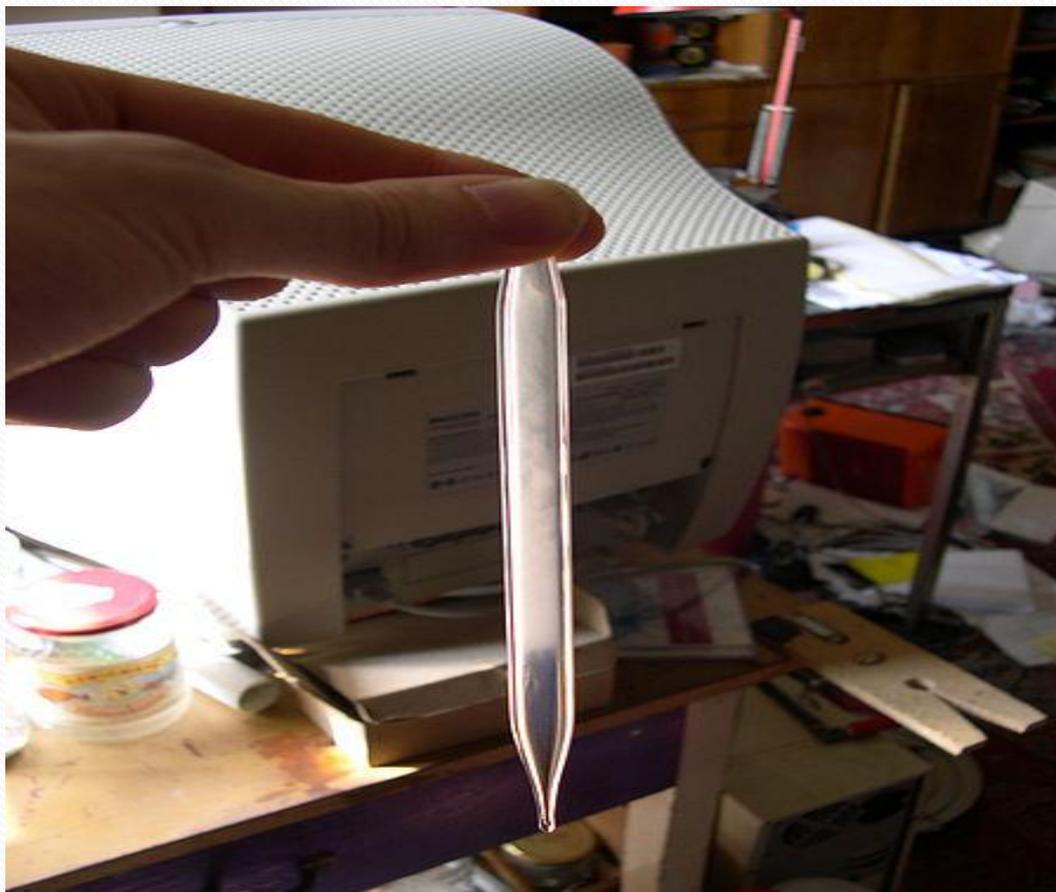
Temperature = 25 °C

5.3 Equations of State for Nonideal Gases:

Run	$T(^{\circ}\text{C})$	$P_{\text{cond}}(\text{atm})$	$\rho_{\text{v}}(\text{kg}/\text{m}^3)$	$\rho_{\text{l}}(\text{kg}/\text{m}^3)$
1	25.0	0.0329	0.0234	997.0
2	100.0	1.00	0.5977	957.9
3	201.4	15.8	8.084	862.8
4	349.8	163	113.3	575.0
5	373.7	217.1	268.1	374.5
6	374.15	218.3	315.5	315.5
7	>374.15	<i>No condensation occurs!</i>		

- ✓ Critical temperature is the highest temperature at which a species can coexist in two phases (liquid and vapor).
- ✓ **Vapor** is a gaseous species below its critical temperature, while **gas** is a species above its critical temperature.

5.3 Equations of State for Nonideal Gases:



5.3b Virial Equations of State:

- ✓ It is a power series expansion for the inverse of specific volume:

$$\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}} + \frac{C}{\hat{V}^2} + \frac{D}{\hat{V}^3} + \dots$$

- ✓ Truncated Virial Equation of State:

$$\frac{P\hat{V}}{RT} = 1 + \frac{B}{\hat{V}}$$

- How to calculate the attached parameters?

$$T_r = \frac{T}{T_c}$$

$$B_o = 0.083 - \frac{0.422}{T_r^{1.6}}$$

$$B_1 = 0.139 - \frac{0.172}{T_r^{4.2}}$$

$$B = \frac{RT_c}{P_c} (B_o + \omega B_1)$$

5.3b Virial Equations of State:

Table 5.3-1 Pitzer Acentric Factors

Compound	Acentric Factor, ω
Ammonia	0.250
Argon	-0.004
Carbon dioxide	0.225
Carbon monoxide	0.049
Chlorine	0.073
Ethane	0.098
Hydrogen sulfide	0.100
Methane	0.008
Methanol	0.559
Nitrogen	0.040
Oxygen	0.021
Propane	0.152
Sulfur dioxide	0.251
Water	0.344

SOURCE: R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids*, 4th Edition, McGraw-Hill, New York, 1986.

5.3b Virial Equations of State:

Example 5.3-1: The truncated Virial Equation

Two gram-moles of nitrogen is placed in a three liter tank -150.8°C . Estimate the tank pressure using ideal gas equation of state and then using the virial equation of state truncated after the second term. Taking the second estimate to be correct, calculate the percentage error that results from the use of the ideal gas equation at the system conditions.

5.3b Cubic Equations of State:

- ✓ They yield a third-order equations upon expansion for the specific volume.
- ✓ Van der Waals equation of state:

$$P = \frac{RT}{\hat{V} - b} - \frac{a}{\hat{V}^2}$$

$$a = \frac{27R^2T_c^2}{64P_c}$$

$$b = \frac{RT_c}{8P_c}$$

5.3b Cubic Equations of State:

✓ Soave-Redlich-Kwong (SRK) equation of state:

$$P = \frac{RT}{\hat{V} - b} - \frac{\alpha a}{\hat{V}(\hat{V} + b)}$$

$$a = 0.42747 \frac{(RT_c)^2}{P_c}$$

$$b = 0.08664 \frac{RT_c}{P_c}$$

$$m = 0.48508 + 1.55171\omega - 0.1561\omega^2$$

$$T_r = \frac{T}{T_c}$$

$$\alpha = \left[1 + m \left(1 - \sqrt{T_r} \right) \right]^2$$

5.3b Cubic Equations of State:

Example 5.3-2: The SRK Equation of State:

A gas cylinder with a volume of 2.50 m^3 contains 1.00 kmol of carbon dioxide at $T=300\text{K}$. Use the SRK equation of state to estimate the gas pressure in atm.

Example 5.3-3: Estimation of Volumes Using the SRK Equation of State:

A stream of propane at temperature $T=423\text{K}$ and pressure $P(\text{atm})$ flows at a rate of 100.0 kmol/h . Use the SRK equation of state to estimate the volumetric flow rate of the stream for $P=0.7 \text{ atm}$, 7.0 atm , 70 atm . In each case, calculate the percentage differences between the predictions of the SRK equation and the ideal gas equation of state.

5.4 The compressibility Factor Equations of State:

- ✓ The compressibility factor of a gaseous species is defined as:

$$z = \frac{P\hat{V}}{RT}$$

- ✓ The compressibility factor equation of state is:

$$P\hat{V} = zRT$$

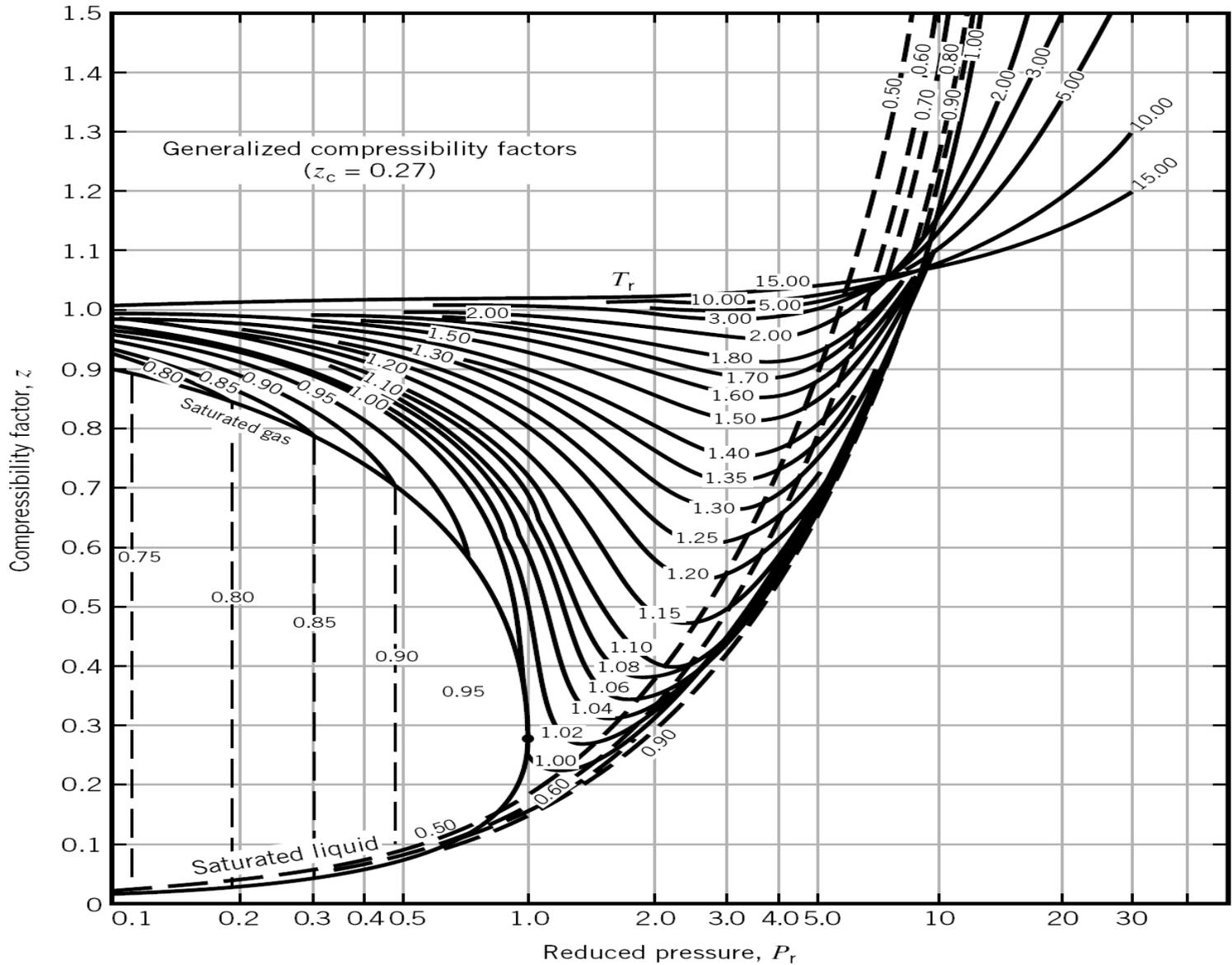
- ✓ The compressibility factor is calculated by:

1. Perry's Chemical Engineers' Handbook as a function of temperature and pressure for a given component.
2. consulting the generalized compressibility charts.

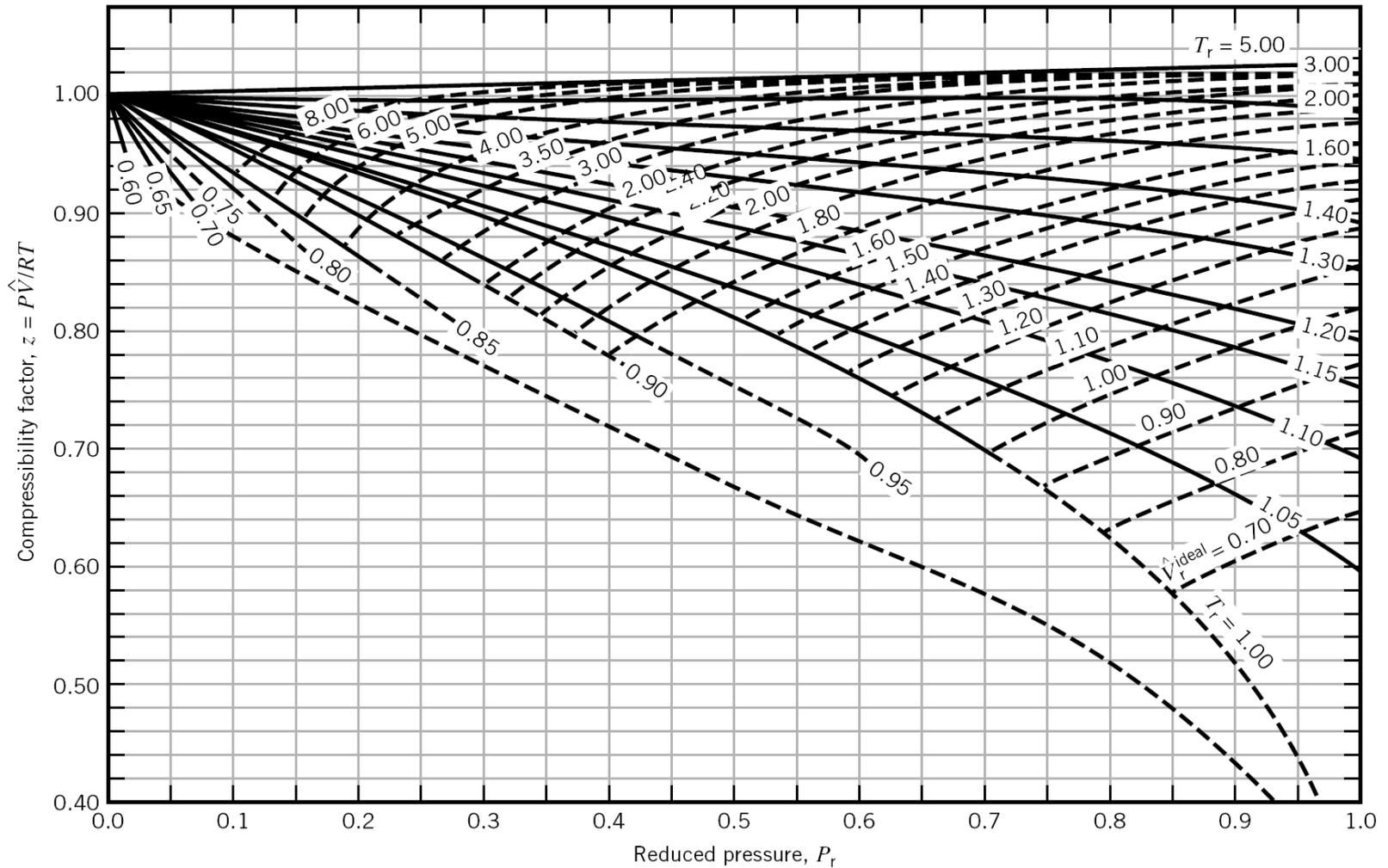
The law of corresponding states:

The value of certain physical properties of a gas, such as compressibility factor, depend to a great extent on the proximity of the gas to its critical state.

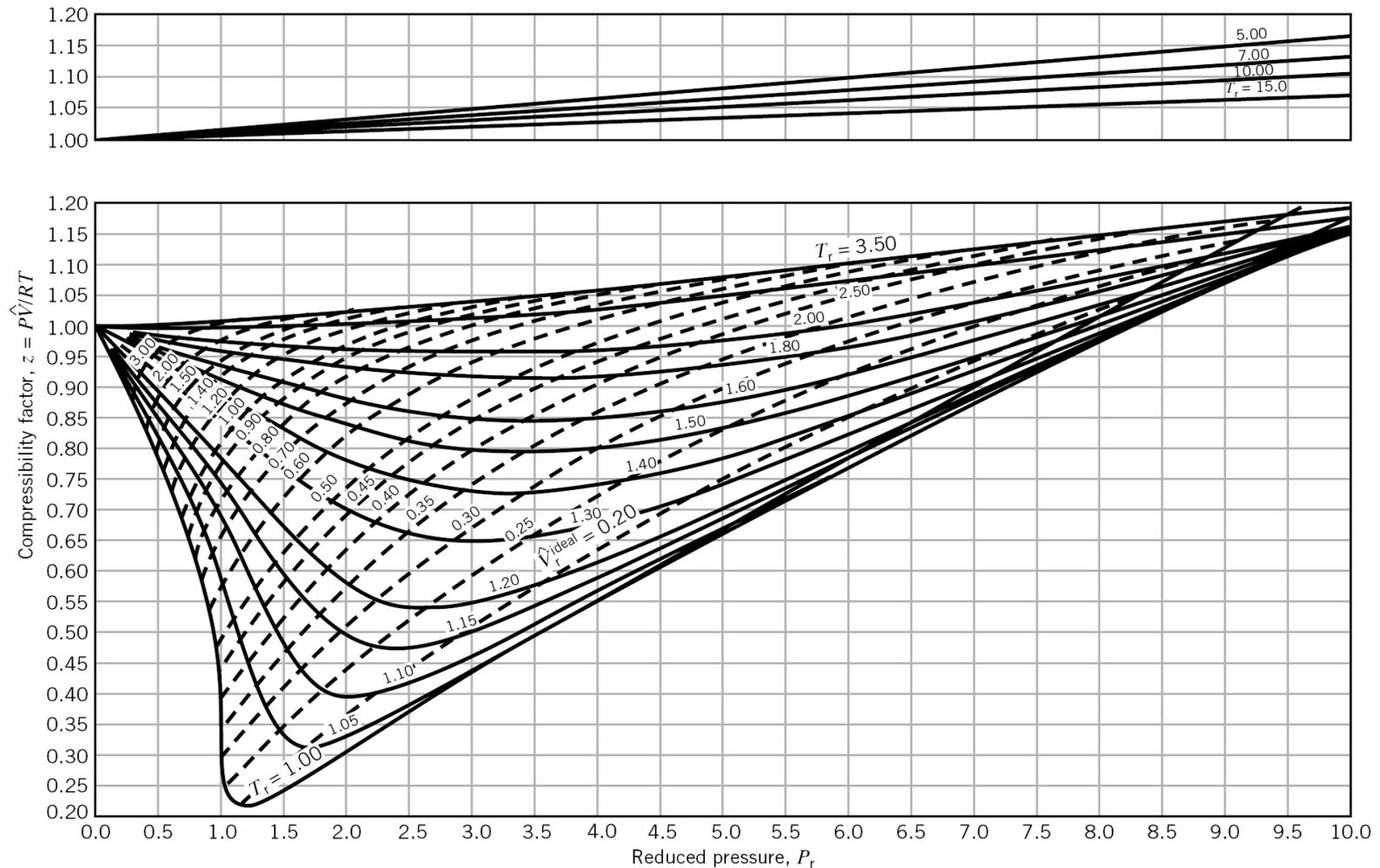
5.4 The compressibility Factor Equations of State:



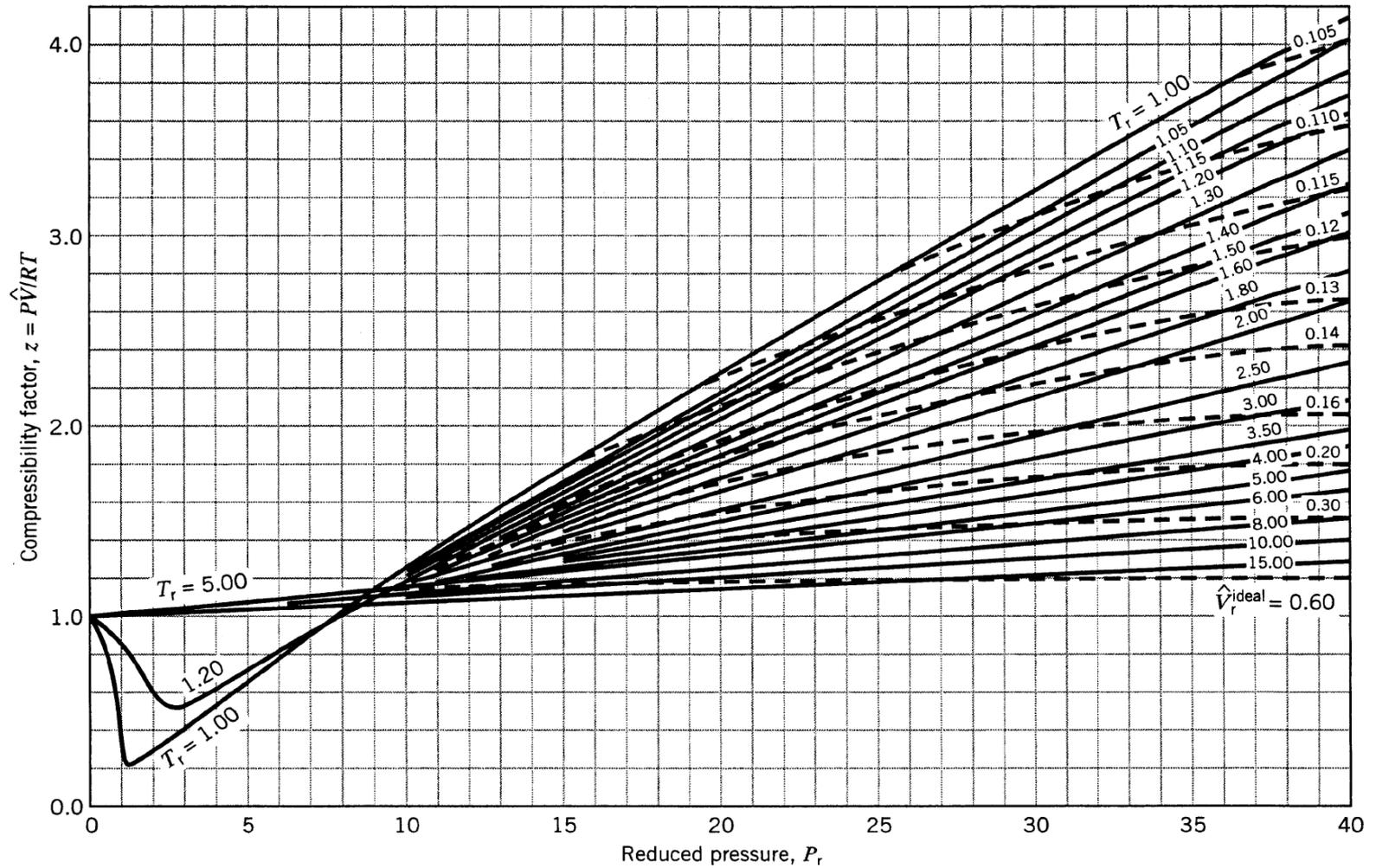
5.4 The compressibility Factor Equations of State:



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5.4 The compressibility Factor Equations of State:



5.4 The compressibility Factor Equations of State:

Procedure for using the generalized compressibility factor:

1. Look up or estimate the critical temperature and critical pressure for the component.
2. If the gas is either hydrogen or helium, adjust the values according to:

$$T_c^a = T_c + 8 K$$

$$P_c^a = P_c + 8 atm$$

which is called Newton's correction.

3. Calculate the reduced values of two known variables (temperature, and pressure, temperature and volume, or pressure and volume) using the definitions:

$$T_r = \frac{T}{T_c}$$

$$P_r = \frac{P}{P_c}$$

$$V_r^{ideal} = \frac{P_c \hat{V}}{RT_c}$$

4. Use the compressibility charts to determine the compressibility factor, and solve for the unknown variable.

5.4 The compressibility Factor Equations of State:

Example 5.4.1: Tabulated Compressibility Factors

Fifty cubic meters per hour of methane flows through a pipeline at 40.0 bar absolute and 300.0 K. Use z from page 2-144 Perry's Chemical Engineers' Handbook to estimate the mass flow rate in kg/h.

5.4 The compressibility Factor Equations of State:

Example 5.4.2: Tabulated Compressibility Factors

One hundred gram-moles of nitrogen is contained in a 5-liter vessel at -20.6°C .

Estimate the pressure in the cylinder.

5.4 The compressibility Factor Equations of State:

✓ **If a gas mixture is involved, Kay's rule is applied.**

✓ **Kay's rule:**

1. Look up the critical temperature and critical pressure for all components involved in the gas mixture.
2. Calculate the Pseudocritical properties of the mixture as simple averages of the component critical constants:

Pesudocritical Temperature: $T'_c = y_A T_{cA} + y_B T_{cB} + y_C T_{cC} + \dots$

Pesudocritical Pressure: $P'_c = y_A P_{cA} + y_B P_{cB} + y_C P_{cC} + \dots$

3. Calculate two variables: the pseudoreduced temperature, pseudoreduced pressure, and pseudoreduced volume of the mixture as:

$$T'_r = \frac{T}{T'_c}$$

$$P'_r = \frac{P}{P'_c}$$

$$\hat{V}_r^{ideal} = \frac{\hat{V} P'_c}{R T'_c}$$

4. Estimate the value of the compressibility factor of the mixture.

5.4 The compressibility Factor Equations of State:

Example 5.4.3: Kay's Rule

A mixture of 75% H₂ and 25% N₂ (molar basis) is contained in a tank at 800 atm and -70°C. Estimate the specific volume of the mixture in L/mol using Kay's rule.

THANK YOU
GO PLEASE AND READ THE LECURE