ABSTRACT

This self-instructional problem workbook is to be used in conjunction with EPA-ATPI Course 503, Accident and Emergency Management. This workbook provides illustrative example problems and solutions dealing with accidents and emergencies. The workbook is divided into four parts: 1) basic operations, dealing with calculations reflecting basic concepts from chemistry, thermodynamics, and physics and which appear in more than one type of application; 2) problems, presenting calculations linked directly with accidents and emergencies; 3) design-oriented applications, concerned with real world industrial problems; and 4) solutions, providing detailed solutions to the problems of the workbook.

Acknowledgement and Disclaimer

Note

EPA policy is to use SI (metric) units only or to list both the common British engineering unit and its SI equivalent. However, British units are primarily used in this manual for the convenience of the majority of the reading audience. Readers more familiar and at ease with SI units are advised to refer to the Appendix IV of this workbook.

Author's Reminder

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Preface

Beginning of the most important part of the work.

Plato(427-327 B.C.)
The Republic, Book I

In recent years, the engineering profession has expanded its responsibilities to society to include accident and emergency management (A&EM), with particular emphasis on emissions from industrial sources. Increasing numbers of engineers, technicians, and maintenance personnel are being confronted with problems in this most important area. The environmental engineer of today and tomorrow must develop a proficiency and an improved understanding of this subject in order to cope with these challenges. Although this is not the first book to treat this particular subject, it is the only problem workbook available for self-study use at this time.

This project was a rather unique undertaking. Rather than prepare a textbook on A&EM in the usual format -- essay material, illustrative examples, nomenclature, bibliography, problems, etc., -- the authors considered writing a self-instructional problem workbook (SIPW). This SIPW would hopefully serve as an adjunct to an A&EM course planned by the EPA's Air Pollution Training Institute. It addresses the problems that will be included in the course to illustrate accident and emergency principles. While this SIPW is to be associated with the A&EM course, it also stands alone as a self-teaching aid.

The authors cannot claim sole authorship to all the problems and material in this SIPW. The present book has evolved from a host of sources, including: notes, homework problems and exam problems prepared by L. Theodore for a one semester, three credit Accident and Emergency Management graduate course at Manhattan College; USEPA APTI Manual "Principles of Accident and Emergency Management"; L. Theodore, J. Reynolds, and F. Taylor's Wiley-Interscience text, "Accident and Emergency Management"; F.P. Lees' Butterworth book (2 volumes) "Loss Prevention in the Process INdustries"; T. A. Kletz's Gulf Publishing text "What Went Wrong?"; C. Springer, J. R. Welker's AICHE notes "Safety, Health and Loss Prevention in Chemical Processing: Undergraduate Instructional Material"; D. B. Turner's USEPA "Workbook of Atmospheric Dispersion Estimates"; USEPA APTI Problem Workbook "Hazardous Waste Incineration", L. Theodore; USEPA APTI Problem Workbook SI:412D "Control of Gaseous and Particulate Emissions", L. Theodore and Y. C. McGuinn; and NESCAUM's (Northeast States for Coordinated Air Use Management) "Air Pollution Control

Inspector's Training Course for the Prevention of Accidental Releases", prepared by Combustion Engineering, Bloomfield, N.J., 1987. Although the bulk of the problems are original and/or taken from sources that the authors have been directly involved with, every effort has been made to acknowledge material drawn from other sources. The authors trust that their apologies will be accepted for any error(s) or omission(s), and changes will be included in a later printing.

INTRODUCTION

This SIPW is divided into four parts: Basic Operations, Problems, Design-oriented Industrial Applications, and Solutions. The first part of the workbook provides a series of basic operations that are required when solving most engineering problems, including those in A&EM. Each basic operation refers to a particular calculation from chemistry, physics, thermodynamics, etc., that many individuals refer to as Basic Concepts. Each operation is presented with a title, problem statement, pertinent data, and solution in programmed instructional format. A COMMENT statement appears with most problems; this often contains more extensive information and details on the basic operation under review. The second part of the book contains problems. This section deals with individual calculations associated with A&EM. There are three problem sets: Plant Applications, Dispersion, and Hazard and Risk Analysis. There are ten problems in each set. Each problem consists of a title, introductory comments, problem statement- including design data and/or information, and solution outline in programmed instructional format. Here again, a COMMENT statement appears with most problems. The third part of the workbook contains two design-oriented problems that deal with real-world industrial applications. Solutions, in part four, are provided for the three problem sets and the two design-oriented problems. An Appendix is also included that contains a discussion of SI units and graphs and tables required for solving the problems in the workbook.

It is hoped that this writing will place in the hands of regulatory agency personnel a workbook covering the principles and applications of accident and emergency management in a thorough and clear manner. Upon completion of the SIPW the reader should have acquired not only a working knowledge of the principles of A&EM but also experience in their application; and, the reader should find himself approaching advanced texts, engineering literature and industrial applications (even unique ones) with more confidence.

Last but not least, we believe that this modest work will help the majority of individuals working in the environmental field to obtain a reasonably complete understanding of A&EM. If you have come this far, and read through the preface, you have more than just a passing interest in A&EM. We strongly suggest you try this SIPW; we think you'll like it.

Theresa Kiernan provided assistance in proofing the typed pages. Our sincere thanks go to Dr. Francis B. Taylor, Department of Mathematics at Manhattan College, for his invaluable help in preparing some of the hazard and risk assessment problems.

Charles Pratt, located in USEPA's Air Pollution Training Institute in Research Triangle Park, NC, deserves special credit for realizing the need for a project of this nature.

Louis Theodore
Young Choi McGuinn

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BASIC OPERATIONS

The Basic Operations section contains 15 basic operations. Each refers to a particular calculation or calculations from chemistry, physics, thermodynamics, etc. The operations are termed basic since they are common to many engineering calculations. These will better assist the reader in grasping the concepts of some of the more detailed calculations that appear later in the workbook.

Each basic operation consists of a problem title, problem statement, pertinent data, and solution in programmed instructional format. These are relatively simple problems; the reader should encounter little difficulty in their solution. Those readers with a strong technical background should proceed directly to the next section (Problems).

BASIC OPERATION 1

Conversion of Units

Given the specific gravity of a liquid, determine its density; convert heat capacity, thermal conductivity and viscosity from SI units to English units.

Specific gravity is the ratio of two densities, that of the substance of interest to that of a reference substance. The reference substance is normally water. The heat conductivity of a substance is defined as the quantity of heat required to raise the temperature of that substance by one degree. Thermal conductivity provides a measure of how fast (or how easily) heat flows through a substance; it is defined as the amount of heat that flows in unit time through a unit area of unit thickness as a result of a unit difference in temperature. The viscosity of a fluid provides a measure of the fluid's resistance to flow.

Data

Specific gravity of liquid (methanol)
= 0.92 (@60 $^{\circ}$F)
Density of reference substance (water @60 $^{\circ}$F)
= 62.4 lb/ft^3
Heat conductivity of methanol
= 0.61 cal/g-$^{\circ}$C (@60 $^{\circ}$F)
Thermal conductivity of methanol
= 0.0512 cal/m-sec-$^{\circ}$C (@60 $^{\circ}$F)
Viscosity of methanol
= 0.64 cp (@60 $^{\circ}$F)

Solution

1. Write the equation describing the definition of specific gravity.

Specific gravity of methanol
= (density of methanol/ density of water)

The density of water is 62.4 lb/ft^3 in English (or Engineering) units and 1.0 g/cm^3 in SI units.

2. Calculate the density of methanol in English units by multiplying the specific gravity by the density of water.

Density of methanol = (specific gravity)(density of water)
= (0.92)(62.4)
= 57.4 lb/ft^3

The procedure is reversed if one is interested in calculating specific gravity from density data. The notation for density is usually ρ.

3. Convert the heat capacity from units of cal/g-°C to Btu/lb-°F.

$$\frac{0.61\ \text{cal}}{\text{g-}^\circ\text{C}}\Big|\frac{454\ \text{g}}{\text{lb}}\Big|\frac{\text{Btu}}{252\ \text{cal}}\Big|\frac{^\circ\text{C}}{1.8\ ^\circ\text{F}}$$

= 0.61 Btu/lb-°F

Note that 1.0 Btu/lb-°F is equivalent to 1.0 cal/g-°C. This also applies on a mole basis, i.e., 1.0 Btu/lbmole-°F = 1.0 cal/gmole-°C.

The usual notation for heat capacity is C_p.

4. Convert the thermal conductivity of methanol to Btu/ft-hr-°F from cal/m-sec-°C.

$$\frac{0.0512\ \text{cal}}{\text{m-sec-}^\circ\text{C}}\Big|\frac{\text{Btu}}{252\ \text{cal}}\Big|\frac{0.3048\ \text{m}}{\text{ft}}\Big|\frac{3600\ \text{sec}}{\text{hr}}\Big|\frac{^\circ\text{C}}{1.8\ ^\circ\text{F}}\Big|$$

= 0.124 Btu/ft-hr-°C.

The factor for converting cal/m-sec-°C to Btu/ft-hr-°F is 2.419.

The usual engineering notation for thermal conductivity is k.

5. Convert viscosity from centipoises to lb/ft-sec.

$$\frac{0.64\ \text{cp}}{}\Big|\frac{6.72 \times 10^{-4}\ \text{lb}}{\text{ft-sec-cp}}\Big|$$

= 4.3×10^{-4} lb/ft-sec

The notation for viscosity is typically μ. The kinematic viscosity, ν , is defined by the ratio of the viscosity to density, i.e., $\nu = \mu/\rho$ with units of $\text{length}^2/\text{time}$.

Comment

Note that the above physical properties are strong function of the temperature but weak functions of the pressure. Interestingly, the viscosity of gases increases with increasing temperature; the viscosity of liquids decreases with an increase in temperature.

BASIC OPERATION 2

Weight Fraction, Mole Fraction, and Average Molecular Weight

Given the weight of each gas in a gas mixture, determine the weight and mole fractions of each component, and the average molecular weight of the mixture.

By definition:

Weight fraction = weight of A/ total weight
Mole fraction = moles of A/ total moles
Moles of A = weight of A/ molecular weight of A

Average molecular weight $= \sum$ (mole fraction)(molecular weight)

Data

A gas mixture contains 20 lb of O_2, 2 lb of SO_2, and 3 lb of SO_3.

Solution

1. Determine the molecular weight of each component.

Molecular weight of O_2 = 32
Molecular weight of SO_2 = 64
Molecular weight of SO_3 = 80

You need atomic weight data to determine the molecular weight. For example, the atomic weight of the oxygen atom (O) is 16, and the molecular weight of the oxygen molecule (O_2) is 32. The atomic weight of sulfur is 32.

2. Calculate the weight fraction of each component.

Compound	Weight		Weight Fraction
O_2	20	20/25 =	0.80
SO_2	2		0.08
SO_3	3		0.12
	25		1.00

The weight percent (%) can be calculated by multiplying the last column by 100.

3. Calculate the mole fraction of each component.

Compound	Weight	Molecular Weight	Moles	Mole Fraction
O_2	20	32	20/32 = 0.6250	0.901
SO_2	2	64	0.0301	0.045
SO_3	3	80	0.0375	0.054
			------	------
			0.6938	1.000

Remember, moles = weight/molecular weight

4. Calculate the molecular weight of the mixture by multiplying the molecular weight by its mole fraction to complete the following table.

Compound	Molecular Weight	Mole Fraction	Weights, lbs
O_2	32	0.901	(32)(0.901) = 28.83
SO_2	64	0.045	2.88
SO_3	80	0.0375	4.32

In a gas, mole percent equals volume percent and vice versa.

5. Calculate the average molecular weight of the gas mixture.

Average molecular weight
= 28.83 + 2.88 + 4.32
= 36.03

The sum of the weights in lbs represents the average molecular weight. This is true since the above calculation is based on 1.0 lbmole of the gas mixture.

Comment

The notation for the mole fraction of a component in a liquid or gas mixture is x and y, respectively. The notation for weight fraction in a liquid or solid is usually w_i.

BASIC OPERATION 3

Pressure Terms

Given the height of a column of liquid whose top is open to the atmosphere, determine the pressure (in various units) exerted at the bottom of the column; calculate the pressure drop and partial pressure of a gas.

Pressure is defined as force per unit area.

Data

Height of column = 2.493 ft
Liquid = mercury (Hg)
Density of Hg = 848.7 lb/ft^3
Atmospheric pressure
= 2116 lb$_f$/ft^2 absolute
Mole fraction of O_2 (in air)
= 0.21

Solution

1. Write an equation describing the gauge pressure in terms of the column height and liquid density.

$$P = \rho gh/g_c$$

where: P = gauge pressure
ρ = liquid density
h = height of column
g = acceleration of gravity
g_c = conversion constant.

This equation is derived by a force balance around the column, the details of which are not given here. The gauge pressure is a pressure term expressed as a quantity above atmospheric pressure (or some other reference pressure).

2. Calculate the pressure in lb$_f$/ft^2 gauge.

$$\begin{aligned} P &= \rho gh/g_c \\ &= (848.7)(1)(2.493) \\ &= 2116 \text{ lb}_f/\text{ft}^2 \text{ gauge} \end{aligned}$$

Note that g/g_c is equal to 1.0 lb/lb$_f$ in engineering units.

3. Determine the pressure in lb_f/ft^2 absolute.

Absolute pressure = guage pressure + atmospheric pressure
= 2116 + 2116
= 4232 lb_f/ft^2 absolute

By definition:
Absolute pressure = gauge pressure + atmospheric pressure. Remember that the atmospheric pressure is the pressure of the air and the atmospheric surroundings while the absolute pressure is a measure of pressure referred to a complete vacuum, or zero pressure. Expressed in various units, the standard atmosphere is equal to:

1.00	Atmospheres (atm)
33.91	Feet of water (ft H_2O)
14.7	Pounds per square inch absolute (psia)
29.92	Inches of mercury (in. Hg)
760.0	Millimeters of mercury (mm Hg)
1.013×10^5	Newtons per square meter (N/m^2)
2116	Pounds per square foot absolute (psfa)
1.0133	Bar

4. Determine the pressure in psia.

psia = (4232 psfa)(1 ft^2/144 in^2)
= 29.4 psia

The corresponding gauge pressure in psi is

psig = 29.4 - 14.7
= 14.7 psig

5. Determine the pressure in mm Hg.

mm Hg = (29.4 psia)(760 mm Hg/14.7 psia)
= 1520 mm Hg

Remember that 760 mm Hg is equal to 14.7 psia which in turn is equal to 1.0 atm.

6. Determine the pressure in in. H_2O.

in. H_2O = (29.4/14.7)(33.91)(12)
= 813.84 in. H_2O

Many pressure terms in engineering applications are expressed in in. H_2O. Correspondingly, pressure drops (or pressure changes) across equipment are also expressed in in. H_2O.

7. Determine the pressure difference (or pressure drop) between the base of the column and atmospheric pressure in in. H_2O.

$$\begin{aligned}\text{in. } H_2O &= 813.84 - (33.91)(12)\\ &= 813.84 - 406.92\\ &= 406.92 \text{ in. } H_2O\end{aligned}$$

Pressure drop, required in many fan and horsepower calculations, represents a pressure difference between two points in a system. Thus, if an inverted U-tube manometer containing water is connected between two different points in a system, and the water level difference in the tube is 32 inches, the pressure drop would be recorded as 32 in. H_2O.

8. Write the equation describing the partial pressure of a component in a gas mixture.

$$p = P\,y$$

where: p = partial pressure
P = pressure of medium
y = mole fraction of component.

Strictly speaking, this equation applies to only ideal gas mixtures. However, it is routinely used in engineering calculations.

9. Calculate the partial pressure of oxygen in the atmosphere.

$$\begin{aligned}p &= P\,y\\ &= (1 \text{ atm})(0.21)\\ &= 0.21 \text{ atm}\end{aligned}$$

Partial pressures may be converted to ppm (parts per million) by multiplying by 10^6. Thus, the ppm of the oxygen in the atmosphere is 21×10^4.

Comment

The reader should note that absolute and gauge pressures are usually expressed with units of atm, psi, or mm Hg. This statement also applies to partial pressures. However, the most common unit employed to describe pressure drop is in. H_2O.

BASIC OPERATION 4

Ideal Gas Law

Given the pressure, temperature, and molecular weight of an ideal gas, determine its density at standard conditions; convert a standard volumetric flow rate to an actual volumetric flow rate.

Data

Pressure = 1.0 atm (standard)
Temperature = 60 °F (standard)
Molecular weight of gas = 29
Standard volumetric flow rate
 for a gas stream = 2000 scfm
Actual operating conditions
= 700 °F and 1 atm.

An ideal gas is an imaginary gas which exactly obeys certain simple laws (ideal gas law). No real gas obeys the ideal gas law exactly, although the "lighter" gases (hydrogen, oxygen, air, etc.) at ambient conditions approach ideal gas law behavior. The "heavier" gases such as sulfur dioxide and hydrocarbons, particularly at high pressures and low temperatures, deviate considerably from the ideal gas law. Despite these deviations, the ideal gas law is routinely used in engineering calculations.

The actual volumetric flow rate, usually expressed in acfm (actual cubic feet per minute), is the volumetric flow rate based on actual operating conditions (temperature and pressure of the system). The standard volumetric flow rate, usually expressed in scfm (standard cubic feet per minute), is the volumetric flow rate based on standard conditions. The standard conditions have to be specified, for there are different sets of standard conditions. For most engineering applications, standard conditions are 60 °F and 1 atm or 32 °F and 1 atm.

Solution

1. Write the ideal gas law.

$$PV = nRT$$

where: P = absolute pressure
V = volume
T = absolute temperature
n = number of moles
R = ideal gas law constant

Absolute temperature (°R or °K) are used in the ideal gas law.

$$°F + 460 = °R$$
$$°C + 273 = °K$$

Absolute pressures must also be employed. See Basic Operation 3.

2. Rewrite the ideal gas law in terms of density, ρ.

$$\rho = m/V = nMW/V = PMW/RT$$

where: MW = molecular weight
m = mass of gas

Remember that the density is defined as the mass divided by the volume. See Basic Operation 1.

3. Calculate the density of the gas using the appropriate value of R.

$$\begin{aligned}\rho &= PMW/RT\\ &= (1)(29)/(0.73)(60+460)\\ &= 0.0764\ \text{lb/ft}^3\end{aligned}$$

Typical values of R are given below:
R = 10.73 psia-ft^3/lbmole-°R
R = 1545 psqf-ft^3/lbmole-°R
R = 0.73 atm-ft^3/lbmole-°R
R = 555 mmHg-ft^3/lbmole-°R
R = 82.06 atm-cm^3/gmole-°K
R = 1.986 cal/gmole-°K
R = 1.986 Btu/lbmole-°R
R = 83.14 mbar-m^3/kmole-°K

The choice of R is arbitrary, provided consistent units are employed.

Since the molecular weight of the given gas is 29, this calculated density may be assumed to apply to air.

4. Combine Boyle's law and Charles' law to relate the actual volumetric flow rate to the standard volumetric flow rate.

$$Q_a = Q_s(T_a/T_s)(P_s/P_a)$$

Charles' law states that the volume of an ideal gas is directly proportional to the temperature at constant pressure. Boyle's law states that the volume of an ideal gas is inversely proportional to the pressure at constant temperature.

where: Q_a = actual volumetric flow rate
Q_s = standard volumetric flow rate
T_s = standard temperature, °K or °R
T_a = actual operating temperautre, °K or °R
P_s = standard pressure, absolute
P_a = actual operating pressure, absolute

5. Calculate the actual volumetric flow rate in acfm.

$$\begin{aligned} Q_a &= Q_s(T_a/T_s) \\ &= 2000(700+460)/(60+460) \\ &= 4462 \text{ acfm} \end{aligned}$$

Remember that absolute temperatures and pressures are used in all ideal gas law calculations. If the pressure is constant, the following equation is used.

$$Q_a = Q_s(T_a/T_s)$$

If it is desired to convert from acfm to scfm, reverse the procedure and use the following equation.

$$Q_s = Q_a(T_s/T_a)(P_a/P_s)$$

Actual flow rates must be used in order to design or predict performance of process equipment.

Comment

The effect of pressure, temperature, and molecular weight on density can be obtained directly from the ideal gas law equation. Increasing the pressure and molecular weight increases the density; increasing the temperature decreases the density.

BASIC OPERATION 5

Discharge Velocity

Given an exhaust gas volumetric flow rate from a stack, calculate the discharge velocity.

The stack discharge velocity is the velocity at which the exhaust gas from a process is discharged to the atmosphere.

Data

Standard volumetric flow rate of exhaust gas = 1000 scfm
Standard conditions = 60 °F and 1.0 atm
Actual temperature of exhaust gas = 300 °F
Diameter of the stack = 1.2 ft

Solution

1. Calculate the actual volumetric flow rate, Q_a.

$$Q_a = Q_s(T_a/T_s)(P_s/P_a)$$

where: Q_a = actual volumetric flow rate
Q_s = standard volumetric flow rate
T_a = actual temperature, °R or °K
T_s = standard temperature, °R or °K
P_a = actual absolute pressure
P_s = standard absolute pressure.

$$Q_a = 1000)[(300+460)/(60+460)](1)$$
$$= 1461.5 \text{ acfm}$$

See Basic Operation 4. Actual volumetric flow rates are always used to calculate the stack discharge velocity. Note that (P_s/P_a) is usually equal to 1.0, since the exhaust gas is discharged to the atmosphere.

2. Calculate the cross-sectional area of the stack, S.

Use the diameter of the stack in the calculation.

$$
\begin{aligned}
S &= \pi D^2/4 \\
&= (\pi)(1.2)^2/4 \\
&= 1.131\ \text{ft}^2
\end{aligned}
$$

3. Calculate the discharge velocity, v.

The velocity calculated here is the bulk, or average, velocity. The average velocity can be simply calculated by dividing the actual volumetric gas flow rate by the cross-sectional area through which the gas flows.

$$
\begin{aligned}
v &= Q_a/S \\
&= (1461.5)/(1.131) \\
&= 1292.2\ \text{ft/min} \\
&= 21.5\ \text{ft/sec}
\end{aligned}
$$

Comment

Inlet and outlet velocities to/from most industrial equipment should be kept at or below 25 ft/sec. It is poor practice to exceed a value of 30 ft/sec, particularly on the inlet side, because of disturbance effects.

BASIC OPERATION 6

Reynolds Number, Re

Given the physical properties and velocity of a gas stream through a circular duct, determine the Reynolds number of the gas stream.

The Reynolds number provides information on flow behavior. Laminar flow is always encountered at a Reynolds number below 2100 in a tube, but it can persist up to Reynolds numbers of several thousand under special conditions. Under ordinary conditions of flow, the flow is turbulent at a Reynolds number above about 4000. Between 2100 and 4000 a transition region is found where the type of flow may be either laminar or turbulent.

Data

Velocity through the duct = 25 ft/sec
Duct diameter = 1.5 ft
Gas viscosity = 1.16×10^{-5} lb/ft-sec
Gas density = 0.075 lb/ft^3

Solution

1. Write the definition of Reynolds number.

$$Re = D\,v\,\rho/\mu$$

where: D = duct diameter
v = velocity
ρ = gas density
μ = gas viscosity

By definition, the Reynolds number is dimensionless.

2. Calculate the Reynolds number of the gas stream.

$$\begin{aligned} Re &= D\,v\,\rho/\mu \\ &= (1.5)(25)(0.075)/(1.16 \times 10^{-5}) \\ &= 2.42 \times 10^{5} \end{aligned}$$

For most engineering applications, one can usually assume turbulent (high Reynolds number) flow.

Comment

The Reynolds number appears in many semi-empirical and empirical equations that involve fluid flow, heat transfer, and mass transfer applications.

BASIC OPERATION 7

Stoichiometry

Given a chemical reaction equation, balance the equation and determine the ratio of reactants to products.

A chemical equation provides a variety of qualitative and quantitative information essential for the calculation of the quantities of reactants reacted and products formed in a chemical process.

Data

The reaction equation for the combustion of butane is shown below.

$$C_4H_{10} + O_2 \dashrightarrow CO_2 + H_2O$$

Solution

1. Balance the above equation.

$$C_4H_{10} + (13/2)O_2 \longrightarrow 4CO_2 + 5H_2O$$

No. of carbons in reactants
= No. of carbons in products
= 4
No. of oxygens in reactants
= No. of oxygens in products
= 13
No. of hydrogens in reactants
= No.of hydrogens in products
= 10

The balanced chemical equation must have the same number of atoms of each element in the reactants and products. For example, given the balanced equation,

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

No. of C's in the reactants
= No. of C's in the products
= 1
No. of O's in the reactants
= No. of O's in the products
= 4
No. of H's in the reactants
= No. of H's in the products
= 4

2. Determine how many moles of CO_2 are formed from 1 mole of C_4H_{10}.

Moles of CO_2 formed = 4

Remember that the chemical equation tells us in terms of moles (not mass) the ratios among reactants and products.

Comment

Although the number of moles on both sides of the equation do not balance, the mass of reactants and products (in line with the conservation of mass) does balance.

BASIC OPERATION 8

Required Heat Rate

Given the mass flow rate of a gas stream and its heat capacity, determine the required heat rate to change the gas stream from one temperature to another.

The first law of thermodynamics provides that energy is conserved. For a flow system, neglecting kinetic and potential effects, the energy transferred, q, to or from the flowing medium is given by the product of the heat capacity and the temperature change of the medium.

Data

Mass flow rate of gas stream,
$m = 1200$ lb/min
Average heat capacity of gas,
$C_p = 0.26$ Btu/lb-°F
Initial temperature,
$T_1 = 200$ °F
Final temperature,
$T_2 = 1200$ °F

Solution

1. Write the equation describing the required heat rate, q.

$$\begin{aligned} q &= m\ C_p \Delta T \\ &= m\ C_p(T_2 - T_1) \end{aligned}$$

The required heat rate, q, can also be expressed in terms of enthalpy.

$$q = m \Delta H$$

where: ΔH = change in enthalpy between T_1 and T_2, Btu/lb

Note that if the enthalpy is given with units of Btu/lbmole, the molar flow rate instead of the mass flow rate needs to be used.

2. Calculate the required heat rate, q, in Btu/min.

$$\begin{aligned} q &= m\ C_p(T_2 - T_1) \\ &= (1200)(0.26)(1200-200) \\ &= 3.12 \times 10^5 \text{ Btu/min} \end{aligned}$$

This calculation is based on adiabatic conditions, i.e., the entire heat load is transferred to the flowing gas. The unit is assumed to be perfectly insulated so that no heat is transferred to the surroundings.

Comment

For more complex systems that may include a chemical or combustion reaction, an enthalpy balance is applied across the entire unit or process. The enthalpy of the feed stream(s) is added to the net heating value of the material(s) combusted. This is equated with the enthalpy of the product stream(s) plus the heat loss from the process. All the enthalpy terms must be based on the same reference temperature. Enthalpy has two key properties that should be kept in mind.

1. Enthalpy is a point function, i.e., the enthalpy change from one state (say 200 °F, 1 atm) to another state (say 400 °F, 1 atm) is a function only of the two states and not the path of the process associated with the change.
2. Absolute values of enthalpy are not important. The enthalpy of water at 60 °F, 1 atm, as recorded in some steam tables is zero Btu/lbmole. Another table indicates a value of 224.2. Both are correct! Note that changing the temperature of water from 60 °F to 100 °F results in the same change in enthalpy using either table.

Enthalpy changes may be obtained with units (English) of Btu, Btu/lb, Btu/lbmole, Btu/scf or Btu/time depending on the available data and calculation required.

BASIC OPERATION 9

Gross Heating Value

Given a gas mixture, determine its gross heating value, HV_G.

The gross heating value (HV_G) represents the enthalpy change or heat released when a gas is stoichiometrically combusted at 60 °F, with the final (flue) product at 60 °F and any water present in the liquid state. Stoichiometric combustion requires that no oxygen be present in the flue gas following combustion of the hydrocarbons.

Data

Composition (mole faction) of the gas mixture:

N_2	0.0515
CH_4	0.8111
C_2H_6	0.0967
C_3H_8	0.0351
C_4H_{10}	0.0056
	1.0000

Combustion properties (gross heating value, Btu/scf):

N_2	0
CH_4	1013
C_2H_6	1792
C_3H_8	2590
C_4H_{10}	3370

Solution

1. Set up the following table.

Component	HV_G (Btu/scf)	x_i
N_2	0	0.0515
CH_4	1013	0.8111
C_2H_6	1792	0.0967
C_3H_8	2590	0.0351
C_4H_{10}	3370	0.0056

The gas described in this example is typical of natural gas.

2. Calculate the gross heating value of the gas mixture, HV_G in Btu/scf.

$$HV_G = (0.0515)(0) + (0.8111)(1013) + (0.0967)(1792) + (0.0351)(2590) + (0.0056)(3370)$$

$$= 1105 \text{ Btu/scf}$$

Use the equation

$$HV_G = \sum_{i=1}^{n} x_i \, HV_{Gi}$$

where: x_i = mole fraction of ith component

Comment

The net heating value (HV_N) is similar to HV_G except the water is in the vapor state. The net heating value is also known as the lower heating value and the gross heating value is also known as the higher heating value.

BASIC OPERATION 10

Henry's Law

Given Henry's law constant and the partial pressure of a solute, determine the maximum mole fraction of solute that can be dissolved in solution.

Henry's law states that the partial pressure of a solute in equilibrium in a solution is proportional to its mole fraction in the limit of zero concentration. In environmental or safety applications, the solute refers to the pollutant or toxic.

Data

Partial pressure of H_2S
  = 0.01 atm
Total pressure = 1.0 atm
Temperature = 60 °F
Henry's law constant
  = 483 atm/mole fraction
    (1 atm, 60 °F)

Solution

1. Write the equation describing Henry's law.

$$p_{H2S} = H x$$

where: p_{H2S} = partial pressure of H_2S, atm
H = Henry's law constant, atm/mole fraction
x = mole fraction of H_2S in solution

For an ideal gas, the partial pressure of a component in a gas mixture is given by:

$$p_{H2S} = y_{H2S}\, P$$

where: P = total pressure
y_{H2S} = mole fraction of H_2S in gas mixture

If Henry's law constant is given in dimensionless form, the following equation is used.

$$y = mx$$

where: y = mole fraction of solute in gas
x = mole fraction of solute dissolved in solution
m = Henry's law constant, dimensionless

See also Basic Operation 3.

2. Calculate the maximum mole fraction of H_2S that can be dissolved in solution.

$$\begin{aligned} x_{H2S} &= p_{H2S}/H \\ &= 0.01/483 \\ &= 2.07 \text{ X } 10^{-5} \end{aligned}$$

This maximum mole fraction represents the amount of solute in the liquid in **equilibrium** with its partial pressure.

Comment

Henry's law constant is a strong function of temperature. Henry's law may be assumed to apply for most dilute solutions. This law finds widespread use in absorber calculations since the concentration of the solute in most process gas streams is dilute.

BASIC OPERATION 11

Chemical Reaction Equilibrium

Given the chemical reaction equilibrium constant for a reaction, calculate the equilibrium partial pressure of the participating species.

With regard to chemical reactions, there are two important questions that are of concern to the engineer: (1) how **far** will the reaction go; and (2) how **fast** will the reaction go? Chemical thermodynamics (reaction equilibrium principles) provides the answer to the first equation; however, it tells nothing about the second. Reaction rates fall within the domain of chemical kinetics and will be treated in Basic Operation 12.

Data

Operating pressure = 1 atm
Operating temperature
= 1950 °F
Chemical reaction equilibrium constant (1 atm, 1950 °F)
= 0.112 $atm^{(-0.5)}$
Reaction equation;
$SO_2 + 0.5\ O_2 = SO_3$
Partial pressure of SO_2, O_2
= 0.0006 atm, 0.039 atm, respectively.

Solution

1. Write the chemical reaction equilibrium constant, K, for the reaction,

$$SO_2 + 0.5\ O_2 = SO_3$$

$$K = p_{SO3}/[(p_{O2})^{0.5}(p_{SO2})]$$

where: p = partial pressure, atm

Note that the chemical reaction equilibrium constant is related to the stoichiometric equation. In effect, the K for the reaction $2\ SO_2 + O_2 = 2\ SO_3$ is different from that given here.

2. Calculate the equilibrium partial pressure of SO_3 from the equation.

$$\begin{aligned} p_{SO3} &= (p_{SO2})(p_{O2})^{0.5}\ K \\ &= (0.0006)(0.039)^{0.5}(0.112) \\ &= 1.33\ X\ 10^{-5}\ \text{atm} \end{aligned}$$

Strictly speaking, the SO_2 and O_2 partial pressures employed above should be corrected, since some small quantity is reacted to form SO_3. However, this iterative calculation is hard to justify based on engineering grounds with such a small quantity of SO_3 produced.

3. Determine the ppm of the SO_3 in the gas assuming the system is at atmospheric pressure.

$$\begin{aligned} \text{ppm of } SO_3 &= (p_{SO3})(10^6) \\ &= 1.33X10^{-5}(10^6) \\ &= 13.3\ \text{ppm} \end{aligned}$$

See Basic Operation 3.

Comment

The literature provides numerical values and equations for K as a function of temperature for a variety of other reactions.

BASIC OPERATION 12

Chemical Kinetics

Calculate the time required to achieve a given conversion for a reactor operating at a particular temperature; define first order reactions; define the Arrhenius equation.

Chemical kinetics involves the study of reaction rates and the variables that affect these rates. It is a topic that is critical for the analysis of reacting systems. The rate of a chemical reaction can be described in any of several different ways. The most commonly used definition involves the time rate of change of the amount of one of the components participating in the reaction; this rate is usually based on some arbitrary factor related to the reacting system size or geometry, such as volume, mass, or interfacial area.

Data

Compound = benzene
Conversion = 99.99 %
Operating temperature = 980 °C
Arrhenius constant for frequency factor (A) = 3.3×10^{10} sec
Arrhenius constant for activation energy (E) = 35,900 cal/gmole

Solution

1. Write the kinetic equation for a first order reaction.

$$dC/dt = - kC$$

where: C = concentration of the compound undergoing reaction
k = reaction rate constant
t = time

Many chemical reactions have been shown to be satisfactorily described by a first order reaction.

2. The solution to the above differential equation becomes,

$$\ln(C/C_0) = -k\,t$$

The initial concentration is C_0.

3. Calculate the ratio C/C_0.

$$C/C_0 = (0.0001)/(1.0)$$
$$= 0.0001$$

The conversion is 99.99%.

4. Calculate the reaction rate constant, k, from the Arrhenius equation.

$$k = A\exp(-E/RT)$$
$$= 3.3X10^{10}\exp[-35900/(1.987)(980+273)]$$
$$= 1.79 \text{ X } 10^{4} \text{ sec}^{-1}$$

The temperature dependence of k is given by the Arrhenius equation:

$$k = A\exp(-E/RT)$$

where: A = frequency factor, units of time
E = activation energy, cal/gmole
R = 1.987 cal/gmole-°K
T = temperature, °K.

5. Calculate the required residence time, t.

$$t = -\ln(C/C_0)/k$$
$$= -\ln(0.0001)/1.79X10^{4}$$
$$= 5.14 \text{ X } 10^{-4} \text{ sec}$$

This equation only applies to a first order irreversible reaction.

Comment

Note that all real and naturally occurring reactions are reversible. A **reversible** reaction is one in which the products also react to form the reactants. Unlike **irreversible** reactions that proceed to the right until completion, reversible reactions achieve an equilibrium state after an infinite period of time, so that reactants and products are still present in the system. At this equilibrium state the net reaction rate is zero.

BASIC OPERATION 13

Molecular Diffusion

Give the molecular diffusivity of a vapor (or gas) in air, calculate the molar flux of the vapor.

Mass transfer is important in many areas of science and engineering. One mechanism of mass transfer, defined as molecular diffusion, occurs when one component in a mixture migrates in the same phase or from phase to phase because of a difference in concentration (or partial pressure) between two points.

Data

Molecular diffusivity of toluene in air
$= 0.86 \times 10^{-5}$ m^2/sec
Partial pressure of toluene at point 1 = 700 mbar
Partial pressure of toluene at point 2 = 400 mbar
Distance separating point 1 and 2 = 10 cm
Temperature = 25.9 °C

Solution

1. Write describing the equation for equimolar counter diffusion.

$$N_A = [D_{AB}/(RTZ)](p_{A1} - p_{A2})$$

A consistent set of units for this equation is:

N_A = molar flux of component A, kmole/sec-m^2
D_{AB} = molecular diffusivity of toluene, m^2/sec
T = temperature, °K
Z = point spacing, m
R = ideal gas law constant, 83.14 mbar-m^3/kmole-°K
p = partial pressure, mbar

2. Set the distance separating the two point, Z, in units of meters.

$$Z = 0.1 \text{ m}$$

The units of the terms in the equation must be dimensionally consistent.

3. Set the temperature term in units of degree Kelvin.

$$T = 25.9 + 273$$
$$= 289.9\ ^{o}K$$

Again, all the terms in the above equation must be dimensionally consistent.

4. Substitute into the above equation and calculate the molar flux, N_A.

$$N_A = [(0.86X10^{-5})/(83.14)(298.9)(0.1)](700-400)$$
$$= 1.06X10^{-6}\ kmole/sec\text{-}m^2$$

The calculational procedure can be reversed if flux data is available and information on diffusivity is required.

Comment

All three main types of rate transfer processes (momentum transfer, heat transfer, and mass transfer) are characterized in an elementary sense by the same general type of equation. The transfer of electric current can also be included in this category. This basic equation is as follows:

Rate of a transfer process = Driving force/Resistance

This equation states that in order to transfer a property such as heat or mass, one needs a driving force to overcome the resistance. This is quite similar to Ohm's law in physics, where the flow of electric current is proportional to the voltage drop (driving force) and inversely proportional to the resistance of the conductor. The transfer of heat by conduction also follows this basic equation and is written as Fourier's law for heat conduction in fluids or solids:

$$q_x/A = -k\ dT/dx$$

where: q_x = heat transfer rate in x direction
A = cross-sectional area normal to the direction of flow of heat
k = thermal conductivity
T = temperature
x = distance.

The quantity q_x/A is called heat flux. The quantity dT/dx is the temperature gradient in the x direction. The minus sign in the above equation is required because if the heat flow is positive in a given direction, the temperature decreases in this direction (becomes negative).

BASIC OPERATION 14

Decision Trees

Construct a decision tree given a sequence of events.

A decision tree provides a diagrammatic representation of sequences that begin with a so-called initiating event and terminate in one or more consequences.

Data

Date: a husband's anniversary
Decision: buy flowers or do not buy flowers for wife
Consequences (buy flowers): domestic bliss or suspicious wife
Consequences (do not buy flowers): status quo or wife in tears/husband in doghouse

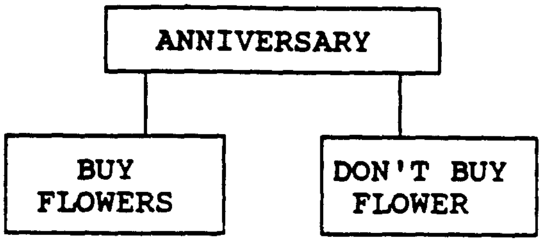
Solution

1. Begin by setting the initial event in "tree" format.

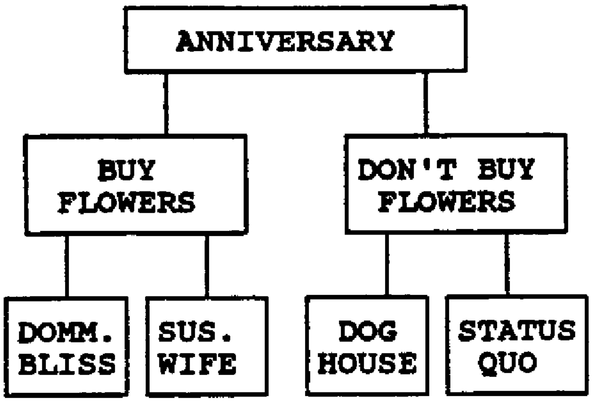
This is often referred to as the top event. Also note that this is an event tree.

2. Set up the first branch from the initial event.

This is the first decision point.



3. Complete the tree.



The bottom four events evolve from what may be defined as resolution of uncertainty points.

Comment

This is an example of an "event" tree. In contrast to a "fault" tree which works backward from a consequence to possible causes, an event tree works forward from the initiating (or top) event to all possible consequences.

BASIC OPERATION 15

Flow Diagram

Prepare a simplified flow diagram for a process.

Before attempting to calculate the raw material or energy requirements of a process it is desirable to attain a clear picture of the process. The best way to do this is to draw a flow diagram. A flow diagram is a line diagram showing the successive steps of a process by indicating the pieces of equipment in the order in which they occur, and the material streams entering and leaving each piece of equipment.

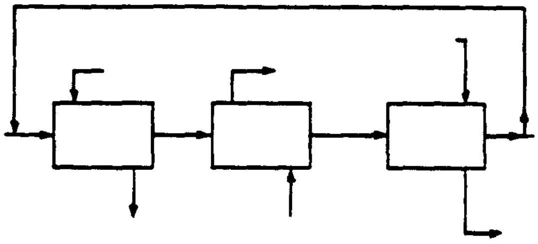
Data

In a process, outside air is mixed with recycled moist air from a dryer (D), and the mixture passes through a heater (H) which uses condensing steam as the heating medium; it then passes through a water spray humidifier (WSH) in which the humidity of the mixture is increased and, finally, through the dryer (D) in which the air acts a drying agent.

Solution

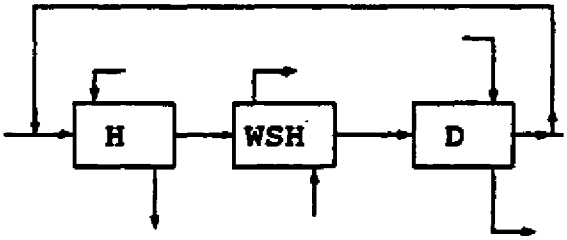
1. First prepare a line diagram of the process.

Lines are usually used to represent streams and boxes may be used to represent equipment.



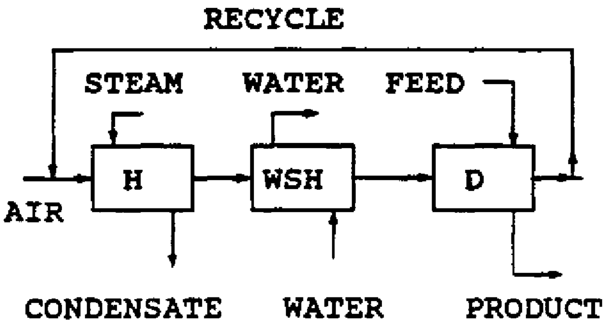
2. Label the equipment.

Notation for individual pieces of equipment is arbitrary.



3. Label the flow streams.

See information provided above.



Comment

In the early 1900's, a new, unifying concept was born. The idea that any and all chemical processes may be resolved into a relatively small number of unit operations and unit processes was proposed. Once quantitative knowledge and effective fundamental theory had been developed for each of these "unit actions," it would be possible to design whole new processes or describe existing processes economically by putting together a coordinated series of scientifically designed **unit actions** regardless of the particular nature of the industry. In other words, filtration is filtration, no matter where you find it, and so on.