

Chemical Engineers are Enhancing Food Production



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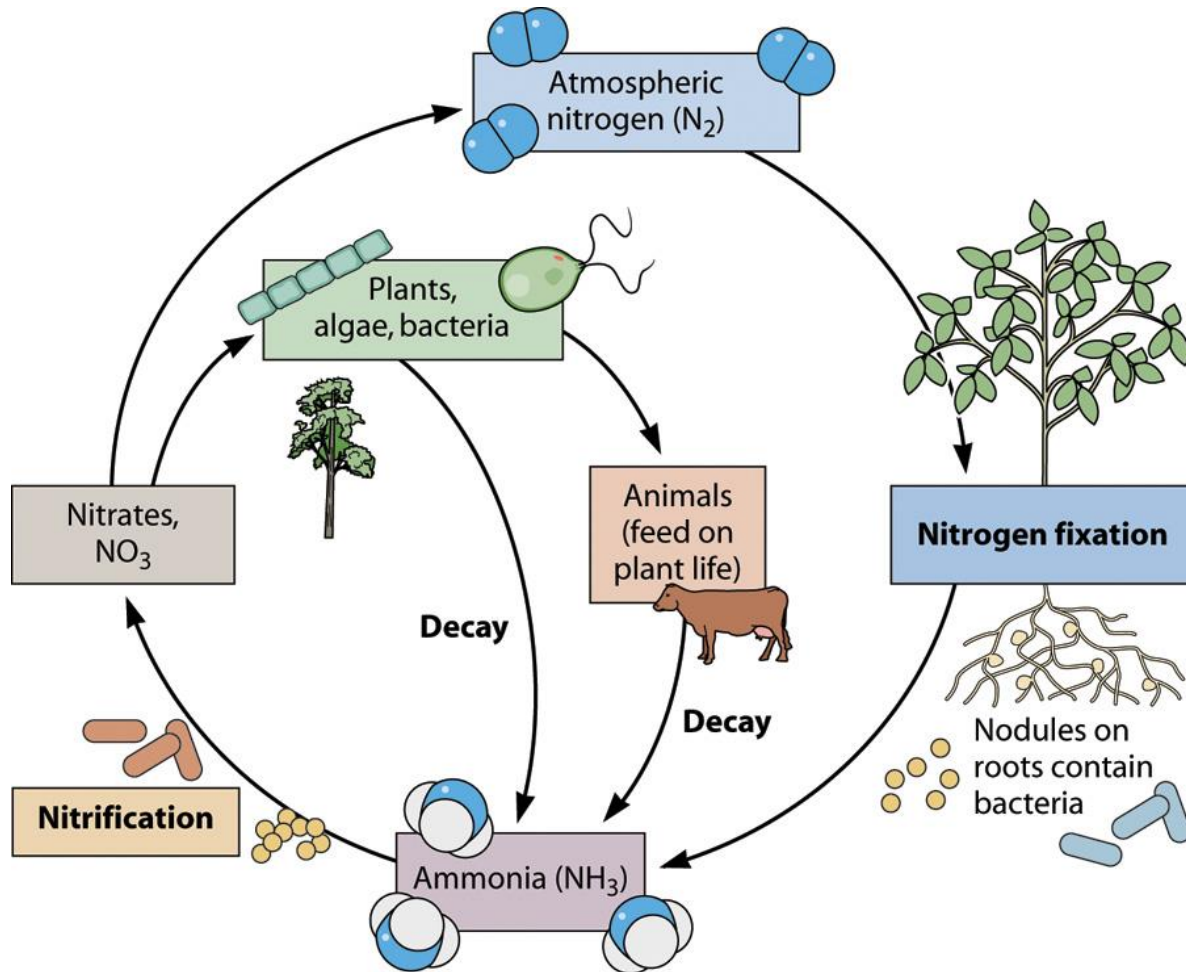
Chemical Engineers' Contribution

- The discovery of **fertilizers**, **pesticides**, and **herbicides**
- Innovations in **food processing** and **packaging** that help improve taste, appearance, and nutritional value while increasing safety, convenience, and shelf life
- New **sterilization** techniques that protect food against spoilage and people against food-borne illnesses.

Fertilizers

- Fritz Haber, a chemist, engineered a process to synthesize ammonia through a reaction between hydrogen and nitrogen in 1908 .
- Nobel Prize in Chemistry in 1918
- Haber-Bosch process
 - Working with Carl Bosch, an industrial chemist, Haber designed and scaled up a successful process for cost-effective commercial-scale production of ammonia for use in nitrogen fertilizers.

Nitrogen Cycle



Nitrogen Cycle

■ Nitrogen fixation

■ Nitrogen-fixing bacteria

- Nitrogenase: $N_2 + 6H_2 \rightarrow 2 NH_3$
- High energy consuming: 15 ~ 20 molecules of ATP

■ Symbiosis between nitrogen-fixing bacteria and plant

- Formation of nodules in plant roots
- Mutual benefits (glucose vs. nitrogen source) : mutualism

■ Chemically synthesized nitrogen fertilizer

- Use high E to break N_2



Pesticides and Herbicides

- Chemical engineers have been instrumental in discovering and synthesizing many chemical compounds that function as pesticides to kill bugs and as herbicides to kill weeds.
- Chemical engineers also design the industrial processes necessary to produce these compounds on a commercial scale.

Herbicides

- Glyphosate
 - the primary ingredient in Monsanto's popular herbicide **Roundup**.
- It works by inhibiting a specific growth enzyme in plants. When applied to crops, glyphosate is rapidly metabolized by weeds.
- Roundup Ready crops
 - Crops genetically modified to be resistant to Roundup
 - Soy, Corn, Canola, Alfalfa, Cotton, Sorghum
Wheat (under development)
 - Referred to as "terminator seeds"

Pesticides

- Chemical pesticides
- Biological pesticides
 - Bt (*Bacillus thuringiensis*) toxin
 - No need to spray synthetic pesticides
 - Not harmful to human and other animals
 - Not kill beneficial insects
 - Traditional pesticides are typically applied only to the leaf and stem (not to the root or inside plant tissues)

Bt Crops



- Bt corn
- Bt potato
- Bt cotton
- Bt soybean

Non-Bt cotton vs. Bt Cotton

Better Foods

- Taste and Look
 - Improving food flavors and textures,
 - Adding nutritional value
 - Perfecting the appearance of foods
- Packaging
 - Modern packaging developed by chemical engineers
- Convenience
 - Fast and easy, delicious and nutritious
 - Fast-cooking foods
 - Frozen foods

Chemical Engineers are Generating Energy



Chemical Engineers are Generating Energy

Chemical Engineers' Contribution

- Traditional, nonrenewable fossil-fuel sources
 - coal, petroleum, natural gas, propane
- Renewable fuels derived from
 - Biomass feedstocks
 - Solar power
 - Wind

Traditional Refining

- Chemical separation and conversion processes to turn crude oil into
 - Gasoline, Diesel and jet fuel, Kerosene, Lubricating oils, Numerous other end products
- Chemical Conversion Processes
 - Thermal cracking
 - Distillation
 - Fluid catalytic cracking
 - Hydrocracking
 - Powerforming

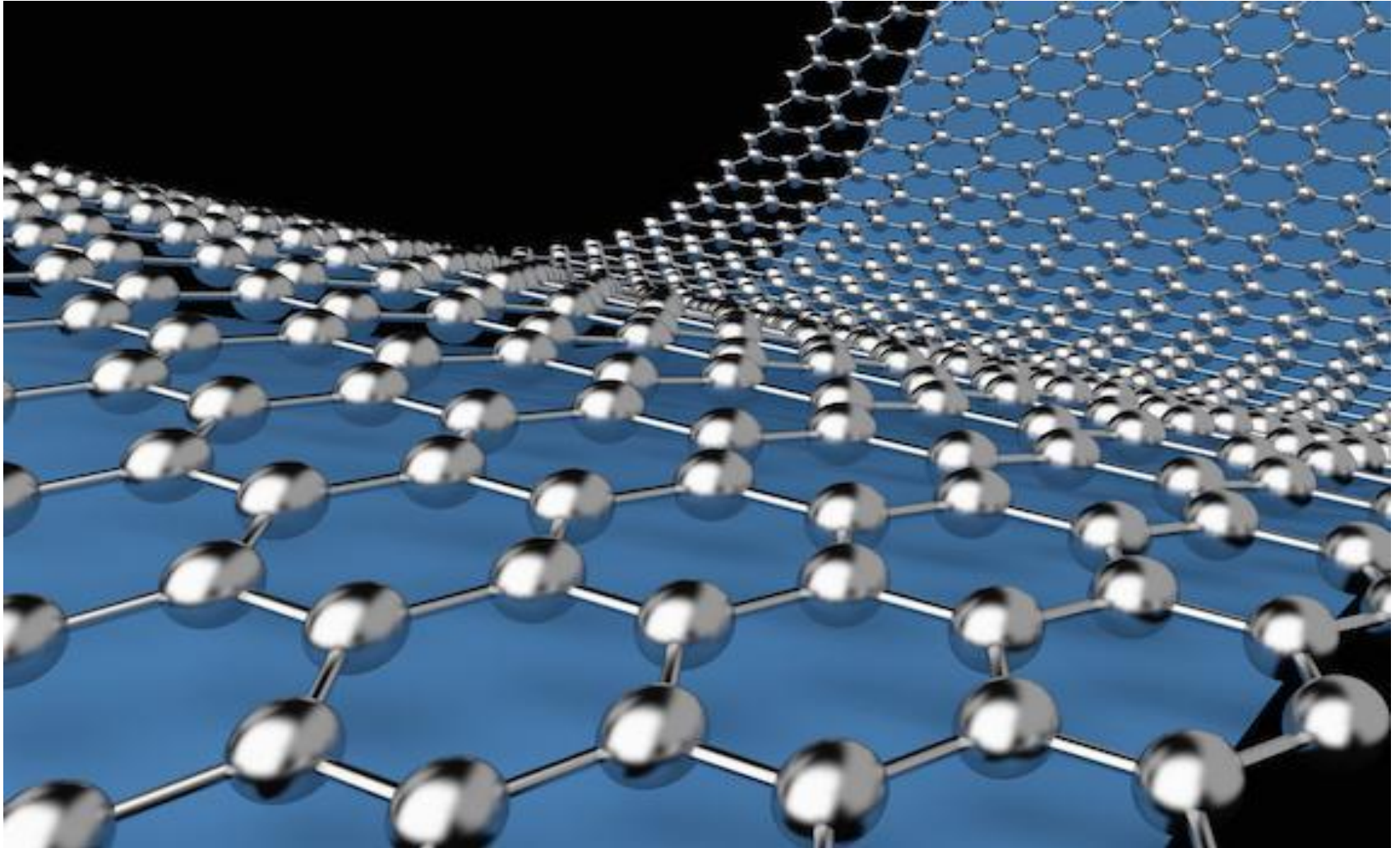
Biofuels & Biorefinery

- Convert renewable biomaterials into electricity and transportation fuels, and valuable chemicals
- Biomass is plant material
 - Fast-growing trees and grasses, grains, corn, sugar cane, wood scrap, even woody leaves and stalks and garbage
 - Sun-dependent renewable feedstock

Biofuels

- **Bioethanol**
 - Made by fermenting biomass rich in carbohydrates (starches and sugars)
 - Gasoline-like alcohol
- **Biodiesel**
 - Made from vegetable oils, animal fat, and even recycled cooking grease
 - Functional alternative to conventional diesel

Chemical Engineers are Improving Materials



Chemical Engineers are Improving Materials

- By manipulating and exploiting the properties, chemical engineers develop and fabricate new end products.
 - Electrical properties
 - Thermal properties
 - Magnetic properties
 - Strength
 - Flexibility or rigidity
 - Resistance to damage.

Plastics

- It was only about 100 years ago that the first true plastic to be commercialized, Bakelite, was invented.
- Composed of long, chain-like molecules produced in a process called polymerization
(Polymer)
 - Broad resistance to chemicals
 - Functional thermal and electrical insulation
 - Light weight with varying degrees of strength
 - Processing flexibility.

Uses of Plastics

- **Everyday uses**
 - children's toys, beverage bottles, clothing, and carpeting and packaging materials
- **More esoteric uses**
 - industrial machine components, automotive parts, biomedical implants, and medical instruments.

Environmentally focused bio-based plastics

- Produced from such renewable raw materials as corn, soybeans, and other agricultural and forest crops
- “Greener” plastics
 - not only help reduce society’s reliance on fossil fuels
 - but are also more biodegradable

Computer Chips

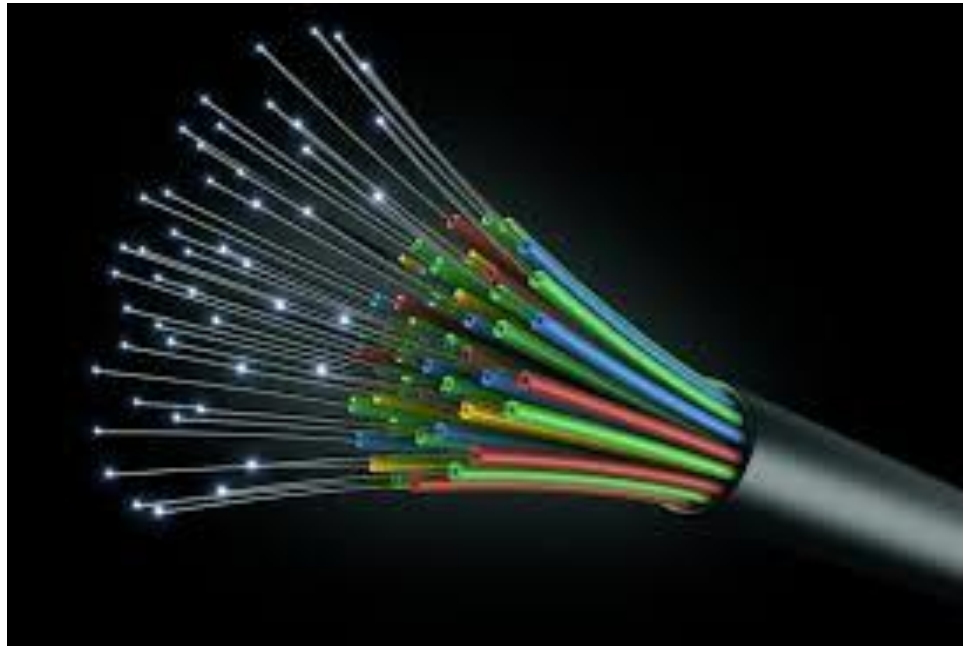
- Electronic devices become smaller, faster, smarter, and cheaper.
- Semiconductor chips
 - provide the backbone for modern computing systems.
 - complex microelectronic circuits composed of a base material with electrical conductivity greater than an insulator but less than a conductor.
 - The typical base material is silicon, although germanium is also used.

Chemical Engineering for Computer Chips

- **Kinetics** and **thermodynamics** in the crystallization of silicon wafers;
- **Polymer science** in the development of patterned photoresist coatings;
- **Heat transfer** to maintain desired temperatures and manage heat buildup during the chip-making process
- **Mass transfer** to improve etching of complex semiconductor-chip patterns and the plating of electronic microchannels.

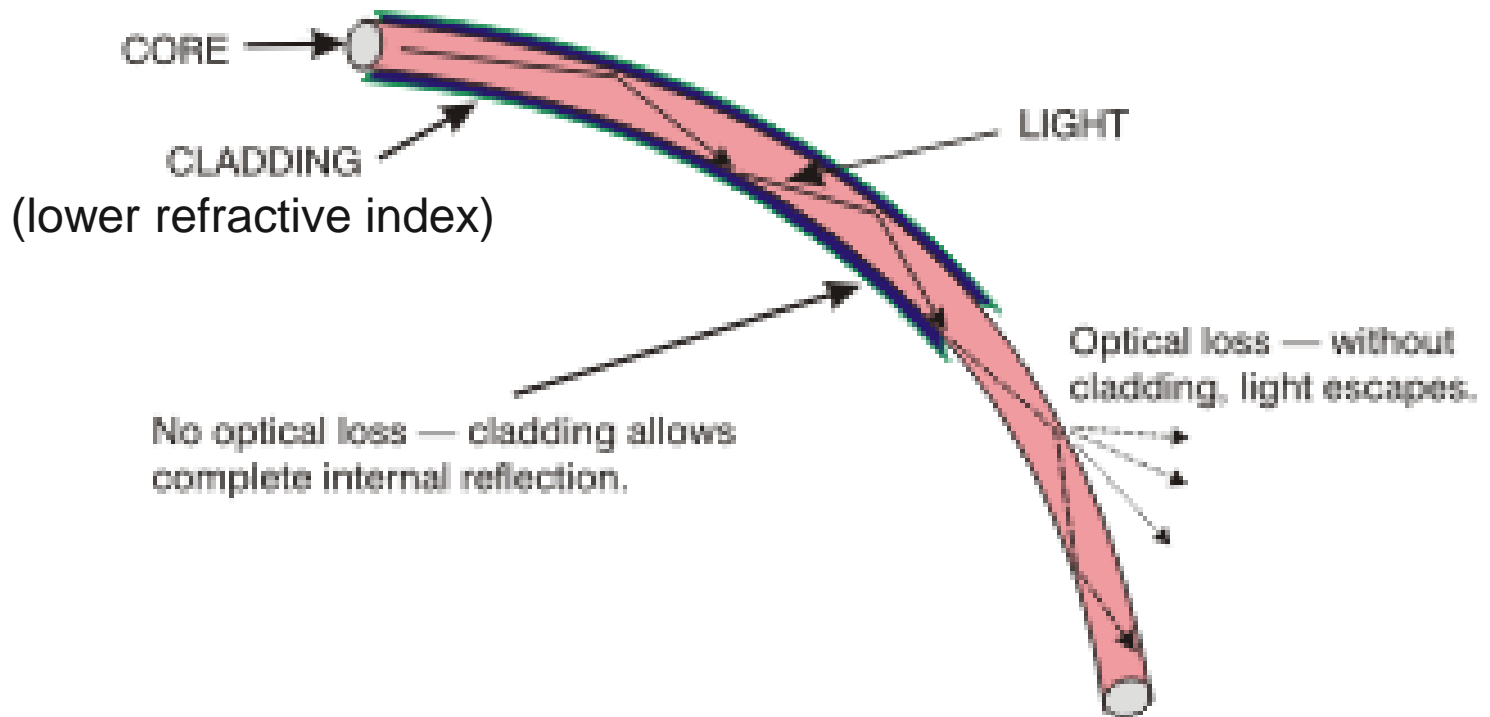
Telecommunications

- Fiber-optic cables
 - Bundles of long, thin glass fibers, each narrower than a human hair



Fiber-optic cables

- Total internal reflection (100% of the light is reflected off the walls of the fiber, so no light is lost)



Fiber-optic cables

- Thin glass fibers are very brittle and fracture easily.
- Modified chemical vapor deposition (MCVD)
 - Chemical engineers invented a process that coats the drawn glass fibers with a specialized polymer.
- This coating
 - maintains the optical properties needed to guide light and data through the fibers
 - prevents the fibers from fracturing, no matter how severely they are bent.

Biomaterials

- Chemical engineers focus their efforts on the discovery and optimization of biocompatible materials.
 - Nontoxic,
 - Well tolerated, and
 - Damage and degradation resistant.

Biomaterials

- Biocompatible materials used inside the body
 - Vascular grafts (specialized polyester)
 - used to repair or reinforce existing veins and arteries
 - Stents (specialized stainless-steel alloys)
 - used to facilitate drainage and reinforce weak arterial tissue
 - Spinal, cardiovascular, and ophthalmic implant devices
 - made from a variety of specialized polymers, ceramics, and metals
 - Artificial knees and hips
 - fabricated from combinations of biocompatible polymers and surgical titanium

Chemical Engineers are Saving the Environment



Chemical Engineers are Saving the Environment

- Chemical engineers develop advanced technologies, monitoring devices, modeling techniques, and operating strategies that
 - Reduce the volume and toxicity of pollutants allowed to enter the air, waterways, and soil;
 - Significantly reduce the negative environmental impact of industrial facilities, power plants, and transportation vehicles; and
 - Allow greater reuse of post-consumer and post-industrial waste streams.

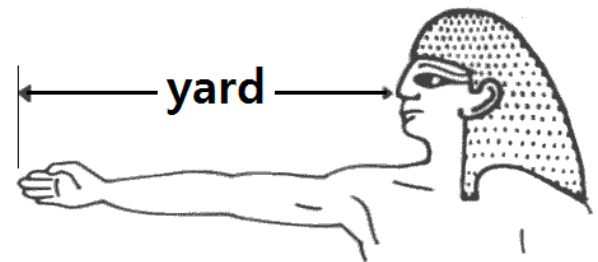
Chapter 4

Describing Physical Quantities



UNITS

- Metric system
 - cgs system: cm, gram, second
 - SI system (Systeme Internationale d'Unites)
- American engineering system
 - Based on cultural definitions from British history
 - e.g. a yard
 - the length from the king's nose to the tip of his middle finger on his fully-extended right arm



UNITS

Table 4.1 Base or Sample Units for Three Measurement Systems

System	Mass	Length	Time	Temperature
cgs	<i>g</i>	<i>cm</i>	<i>s</i>	Celsius
SI	<i>kg</i>	<i>m</i>	<i>s</i>	Kelvin
American	<i>lb_m</i>	<i>ft</i>	<i>s</i>	Fahrenheit

Conversion Factors

Acceleration	$1 \text{ m/s}^2 = 3.2808 \text{ ft/s}^2$	$1 \text{ ft/s}^2 = 0.3048 \text{ m/s}^2$
Area	$1 \text{ cm}^2 = 0.155 \text{ in}^2$	$1 \text{ in}^2 = 6.4516 \text{ cm}^2$
	$1 \text{ m}^2 = 10.764 \text{ ft}^2$	$1 \text{ ft}^2 = 0.092903 \text{ m}^2$
Density	$1 \text{ g/cm}^3 = 62.43 \text{ lb}_m/\text{ft}^3$	$1 \text{ lb}_m/\text{ft}^3 = 0.016019 \text{ g/cm}^3$
	$1 \text{ kg/m}^3 = 0.06243 \text{ lb}_m/\text{ft}^3$	$1 \text{ lb}_m/\text{ft}^3 = 16.019 \text{ kg/m}^3$
Energy	$1 \text{ J} = 0.7376 \text{ ft lb}_f$	$1 \text{ ft lb}_f = 1.3558 \text{ J}$
	$1 \text{ J} = 9.478 \times 10^{-4} \text{ Btu}$	$1 \text{ Btu} = 1055.0 \text{ J} = 778.1 \text{ ft lb}_f$
	$1 \text{ J} = 2.778 \times 10^{-7} \text{ kW hr}$	$1 \text{ kW hr} = 3.600 \times 10^6 \text{ J}$
	$1 \text{ J} = 10^7 \text{ ergs}$	$1 \text{ hp s} = 550 \text{ ft lb}_f$
	$1 \text{ J} = 0.2390 \text{ cal}$	
Force	$1 \text{ N} = 0.22481 \text{ lb}_f$	$1 \text{ lb}_f = 4.4482 \text{ N}$
	$1 \text{ N} = 10^5 \text{ dynes}$	
Length	$1 \text{ cm} = 0.3937 \text{ in}$	$1 \text{ in} = 2.540 \text{ cm}$
	$1 \text{ m} = 3.2808 \text{ ft}$	$1 \text{ ft} = 12 \text{ in} = 0.3048 \text{ m}$
	$1 \text{ km} = 0.6214 \text{ mi (statute)}$	$1 \text{ yd} = 3 \text{ ft}$
	$1 \text{ km} = 0.5400 \text{ nmi (nautical)}$	$1 \text{ mi (statute)} = 1609 \text{ m} = 5280 \text{ ft}$
		$1 \text{ nmi (nautical)} = 1.8520 \text{ km}$
Mass	$1 \text{ g} = 0.03527 \text{ oz}$	$1 \text{ oz} = 28.35 \text{ g}$
	$1 \text{ kg} = 2.2046 \text{ lb}_m$	$1 \text{ lb}_m = 16 \text{ oz} = 453.6 \text{ g}$
	$1 \text{ metric ton} = 1000 \text{ kg} = 2205 \text{ lb}_m$	$1 \text{ ton} = 2000 \text{ lb}_m = 907.2 \text{ kg}$

Conversion Factors

Power	$1 W = 0.7376 \text{ ft lb}_f/s$ $1 W = 9.478 \times 10^{-4} \text{ Btu/s}$ $1 W = 1.341 \times 10^{-3} \text{ hp}$	$1 \text{ ft lb}_f/s = 1.3558 W$ $1 \text{ Btu/s} = 1055.0 W = 778.1 \text{ ft lb}_f/s$ $1 \text{ hp} = 745.7 W = 550 \text{ ft lb}_f/s$
Pressure	$1 Pa = 1.450 \times 10^{-4} \text{ lb}_f/in^2 \text{ (psi)}$ $1 \text{ Torr} = 1 \text{ mm Hg (@ } 0^\circ\text{C)}$	$1 \text{ lb}_f/in^2 = 6894.8 Pa$ $1 \text{ atm} = 101,325 Pa$ $1 \text{ atm} = 760 \text{ mm Hg (@ } 0^\circ\text{C)}$ $1 \text{ atm} = 14.696 \text{ lb}_f/in^2 \text{ (psi)}$ $1 \text{ atm} = 33.9 \text{ ft H}_2\text{O (@ } 4^\circ\text{C)}$
Temperature	$T(^{\circ}\text{C}) = 5/9 [T(^{\circ}\text{F}) - 32]$ $T(\text{K}) = T(^{\circ}\text{C}) + 273.15$	$T(^{\circ}\text{F}) = 1.8 T(^{\circ}\text{C}) + 32$ $T(\text{R}) = T(^{\circ}\text{F}) + 459.67$ $T(\text{R}) = 1.80 T(\text{K})$
Viscosity	$1 \text{ cp} = 6.7197 \times 10^{-4} \text{ lb}_m/\text{ft s}$	$1 \text{ lb}_m/\text{ft s} = 1488.2 \text{ cp} = 14.882 \text{ Poise}$
Volume	$1 \text{ cm}^3 = 1 \text{ mL} = 0.06102 \text{ in}^3$ $1 \text{ m}^3 = 35.3145 \text{ ft}^3$ $1 \text{ m}^3 = 1000 \text{ liters}$ $1 \text{ m}^3 = 264.17 \text{ gal}$ $1 \text{ L} = 0.26417 \text{ gal}$	$1 \text{ in}^3 = 16.387 \text{ cm}^3$ $1 \text{ ft}^3 = 0.028317 \text{ m}^3$ $1 \text{ ft}^3 = 7.4805 \text{ gal}$ $1 \text{ ft}^3 = 28.317 \text{ liters}$ $1 \text{ gal} = 3.785 \times 10^{-3} \text{ m}^3 = 3.785 \text{ L}$
Volume Flow	$1 \text{ m}^3/s = 15,850 \text{ gal/min}$	$1 \text{ gal/min} = 6.309 \times 10^{-5} \text{ m}^3/s$ $1 \text{ gal/min} = 2.228 \times 10^{-3} \text{ ft}^3/s$ $1 \text{ ft}^3/s = 448.8 \text{ gal/min}$

Conversion Factors

$$1 \text{ ft} = 12 \text{ in}, \quad 28 \text{ in} = ? \text{ ft}$$

$$\frac{28 \text{ in}}{1} \times \frac{1 \text{ ft}}{12 \text{ in}} = 2.333 \text{ ft}$$

Moles

- One mole = Avogadro's number of particles
(6.02×10^{23})
- Molecular weight (MW) of H₂O
 $2(1.01) + 16.00 = 18.02$
H O
- gmol (gram-mole)
 - 18 g water = 1 gmol water
- lbmol (pound-mole)
 - 18 lb_m water = 1 lbmol

Symbols

- m = mass
- m_A = mass of “A”
- n = the number of moles
- n_A = the number of moles of “A”
- MW_A = molecular weight of “A”

Combined Units

Table 4.2 Examples of Combined Units for Three Measurement Systems

System	CGS System	SI Systems	American System
density	g/cm^3	kg/m^3	lb_m/ft^3
velocity	cm/s	m/s	ft/s
acceleration	cm/s^2	m/s^2	ft/s^2
volumetric flow rate	cm^3/s	m^3/s	ft^3/s
mass flow rate	g/s	kg/s	lb_m/s
concentration	$gmol/L^*$	$kgmol/m^3$	$lbmol/ft^3$

*often abbreviated M (i.e., molarity)

Force & Defined Units

- Newton's 2nd law

$$F = m a$$

- Weight

$$F_{weight} = m g$$

- lb_m “pound-mass”

- lb_f “pound-force”

Table 4.3 Gravitational Acceleration (at Sea Level) and Defined Units of Force

System	g	Defined Unit of Force
cgs	980.66 cm/s^2	1 <i>dyne</i> \equiv 1 $g\ cm/s^2$
SI	9.8066 m/s^2	1 <i>Newton (N)</i> \equiv 1 $kg\ m/s^2$
American	32.174 ft/s^2	1 <i>pound-force (lb_f)</i> \equiv 32.174 $lb_m\ ft/s^2$

Pressure & Defined Units

- Pressure
 - Force exerted per area
- *psi*
“pound per square inch”

Table 4.4 Commonly Used Units of Pressure

System	Units of Pressure	Abbreviation	Defined and Equivalent Units
cgs	<i>Pascals</i>	<i>Pa</i>	$1 Pa \equiv 1 N/m^2 = 10 g/cm s^2$
SI	<i>kiloPascals</i>	<i>kPa</i>	$1 kPa \equiv 1000 N/m^2 = 1000 kg/m s^2$
American	lb_f/in^2	<i>psi</i>	$1 lb_f/in^2 = 4633 lb_m/ft s^2$

Symbols

- Density

$$\rho = \frac{m}{V}$$

- Flow rate

- mass flow rate (\dot{m})
- molar flow rate (\dot{n})
- volumetric flow rate (\dot{V})

$$\dot{m} = \rho \dot{V}$$

Mixture Composition

- Mole Concentration of A

$$c_A = \frac{\text{moles of A}}{\text{volume of mixture}} = \frac{n_A}{V}$$

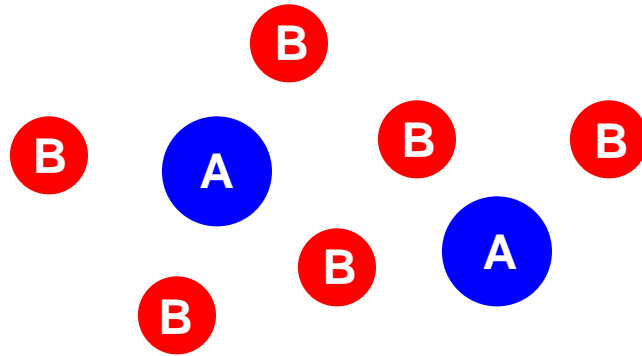
- Mass Fraction of A

$$x_A = \frac{\text{mass of A}}{\text{mass of mixture}} = \frac{m_A}{m}$$

- Mole Fraction of A

$$y_A = \frac{\text{moles of A}}{\text{moles of mixture}} = \frac{n_A}{n}$$

Mole Fraction & Mass Fraction



$$m_A = 2 m_B$$

- Mole Fraction of A = $2/8 = 0.25$
- Mass Fraction of A = $4/10 = 0.4$

Mixture Composition

- Mass Percent of A
(commonly expressed as *wt%*)

$$= 100 x_A$$

- Mole Percent of A

$$= 100 y_A$$

Dimensional Consistency

- Terms that are added together (or subtracted) must have the same units.

$$Q = ab + c^2$$

- Exponents must be unitless.
 - The units in the term ab/c must all cancel out to leave no units.

$$y = x^{ab/c}$$

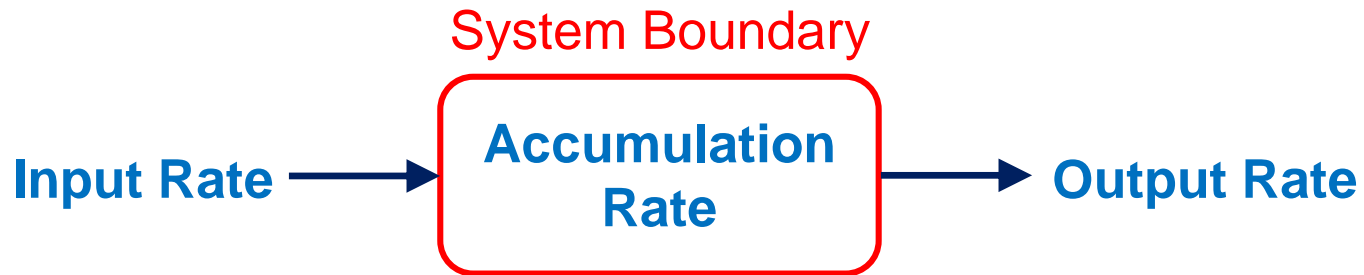
Chapter 5

Material Balances



Conservation of Total Mass

- Total mass is conserved.



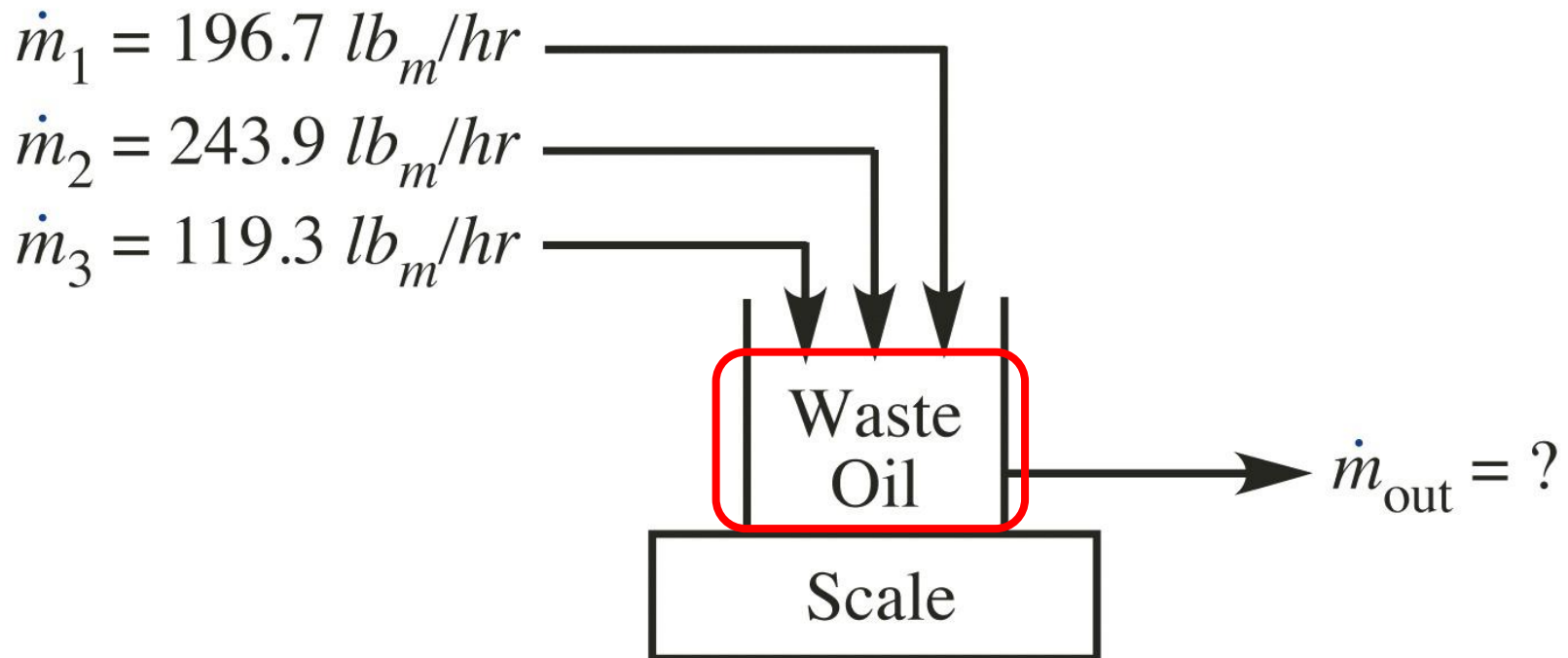
$$\text{Accumulation Rate} = \text{Input Rate} - \text{Output Rate}$$

- When acc. rate = 0, steady-state.

$$\text{Input Rate} = \text{Output Rate}$$

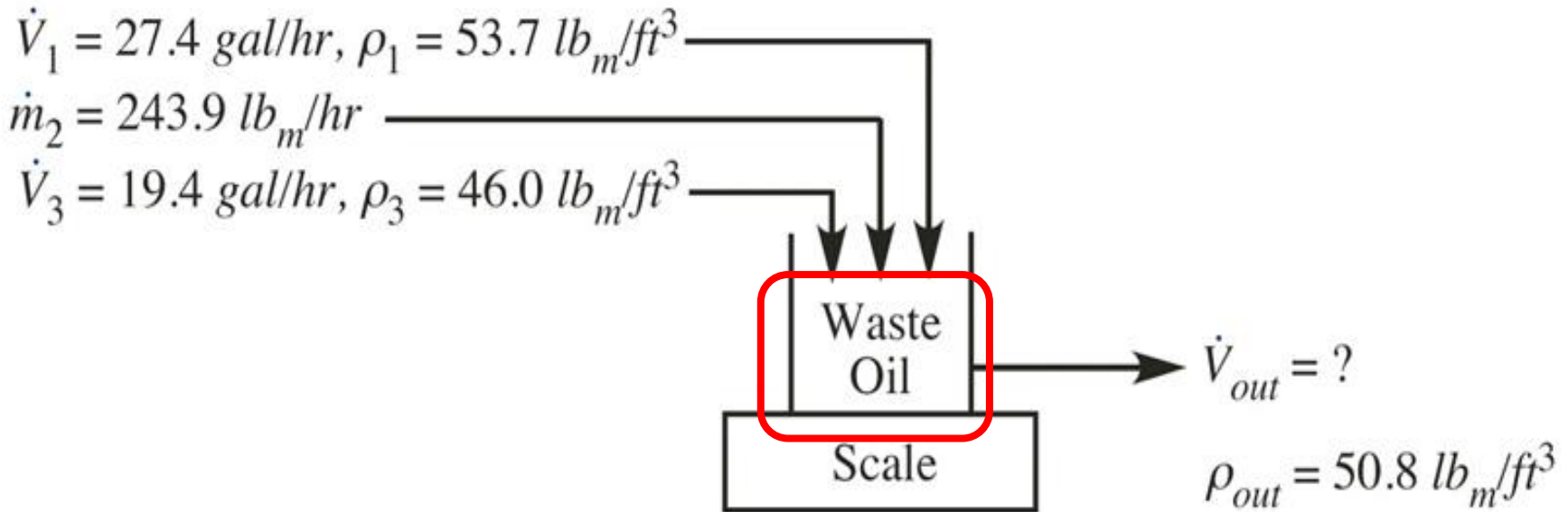
Ex. 5.1. Three different streams deliver contaminated oil to a waste oil tank. At what mass flow rate must the oil be withdrawn to maintain a constant scale reading?

(at steady-state)



Ex. 5.2. At what volumetric flow rate must the oil be withdrawn to maintain a constant scale reading?

(at steady-state)



Example 5.2

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Total Mass Balance

At steady-state

$$\sum_{\substack{\text{inlet} \\ \text{streams}}} \dot{m}_{\text{stream}} = \sum_{\substack{\text{outlet} \\ \text{streams}}} \dot{m}_{\text{stream}}$$

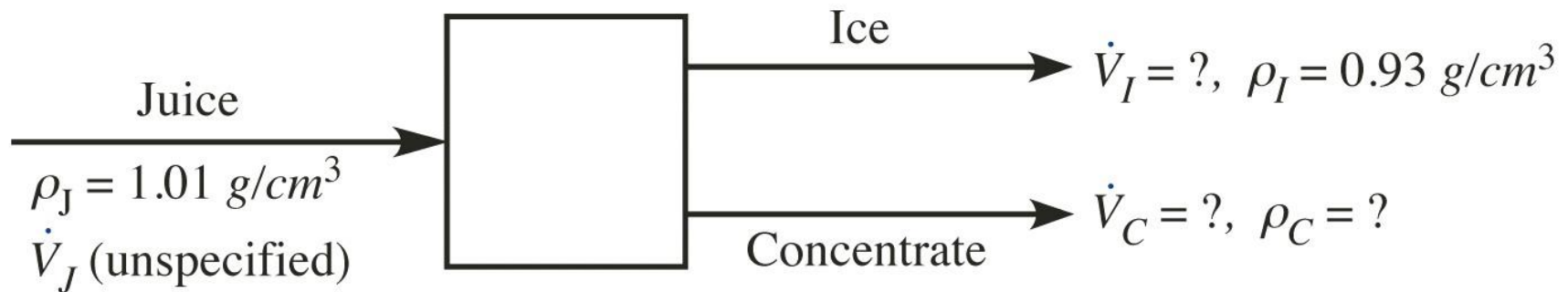
Steps for analyzing material balance problems

- Draw a diagram
- Write all known quantities
- Identify and assign symbols to all unknown quantities
- Select a basis if needed (if no flow rates are known)
- Determine the appropriate set of equations (# of equations = # of unknown)
- Solve algebraically and then numerically

Ex. 5.3. Your company uses a process to concentrate orange juice by freeze drying. What is the density of the concentrate?

Given conditions

$$\dot{V}_C = 0.25 \dot{V}_J \quad \dot{V}_I = 0.7 \frac{\rho_J \dot{V}_J}{\rho_I}$$



Example 5.3

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Conservation of Total Mass

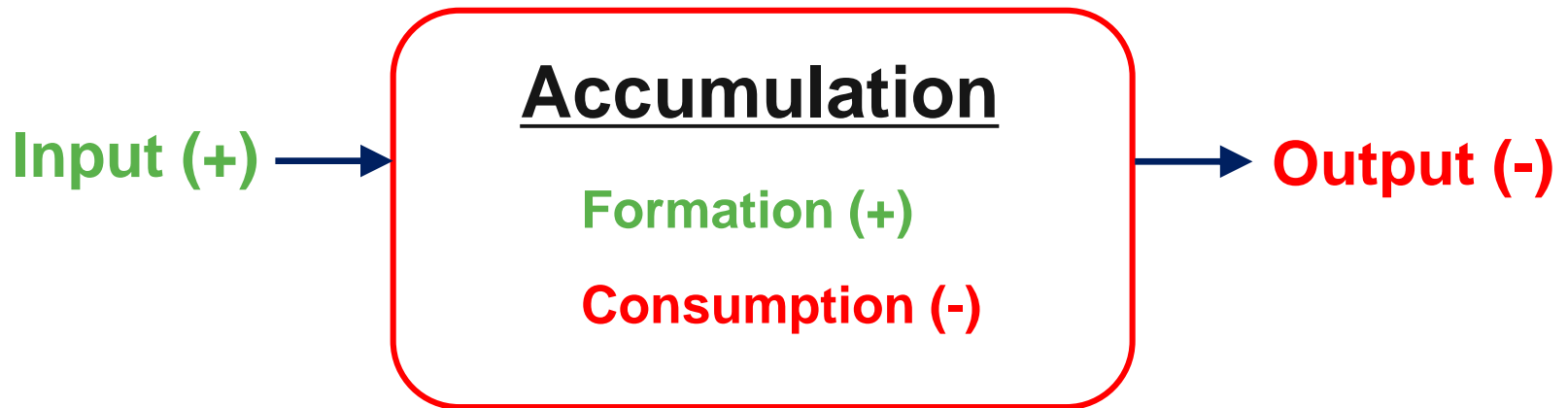
- Unlike total mass, total moles are not always conserved.



- Mass Balance
 - NOT Mole Balance
 - NOT Concentration Balance
 - NOT Volume Balance

Material Balances with Reactions

- Chemical Reactions
 - Formation (= additional input)
 - Consumption (= additional output)



$$\underline{\text{Acc. rate} = \text{In. rate} - \text{Out. rate} + \text{Form. rate} - \text{Con. rate}}$$

Material Balances with Reactions

$$\text{Acc} = \text{In} - \text{Out} + \text{Form} - \text{Con}$$

Accumulation rate

$$= \text{Input rate} - \text{Output rate} \\ + \text{Formation rate} - \text{Consumption rate}$$

$$\frac{d(\quad)}{dt} =$$

Material Balances with Reactions

At steady-state

~~Accumulation rate~~ $\rightarrow 0$

$$= \text{Input rate} - \text{Output rate} \\ + \text{Formation rate} - \text{Consumption rate}$$

$$\text{Input rate} + \text{Formation rate} \\ = \text{Output rate} + \text{Consumption rate}$$

Material Balances for Multiple Species

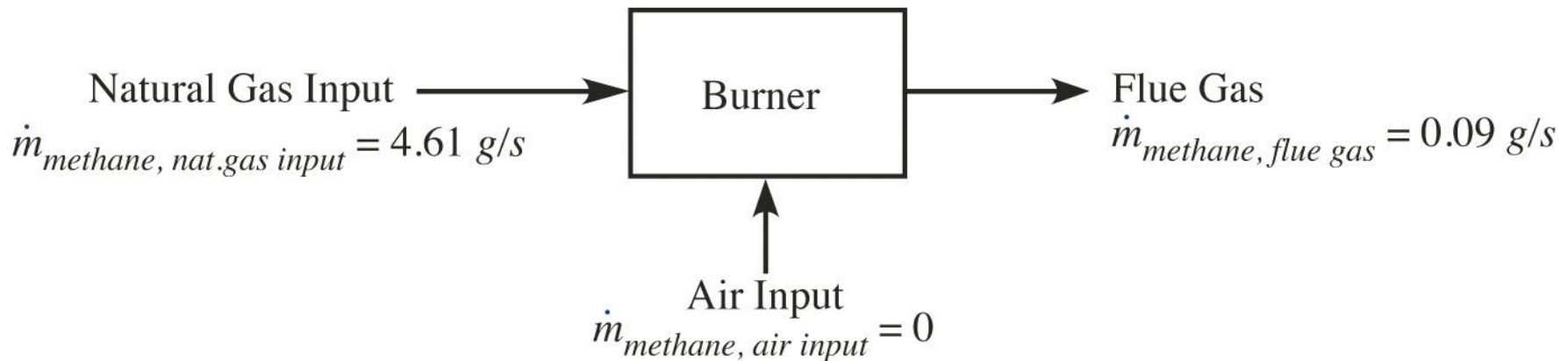
Mass of **Species A** at steady-state:

$$\sum_{\substack{\text{inlet} \\ \text{streams}}} \dot{m}_{A,\text{stream}} + R_{\text{formation},A} = \sum_{\substack{\text{outlet} \\ \text{streams}}} \dot{m}_{A,\text{stream}} + R_{\text{consumption},A}$$

$$\dot{m}_A = x_A \dot{m} = MW_A \dot{n}_A = MW_A y_A \dot{n} = MW_A c_A \dot{V}$$

$$\dot{n}_A = \frac{\dot{m}_A}{MW_A} = \frac{x_A \dot{m}}{MW_A} = y_A \dot{n} = c_A \dot{V}$$

Ex. 5.4. Natural gas, which is essentially pure methane, undergoes steady-state combustion by injecting it into a small burner into which air is also injected. At what rate is the methane being burned (consumed)?

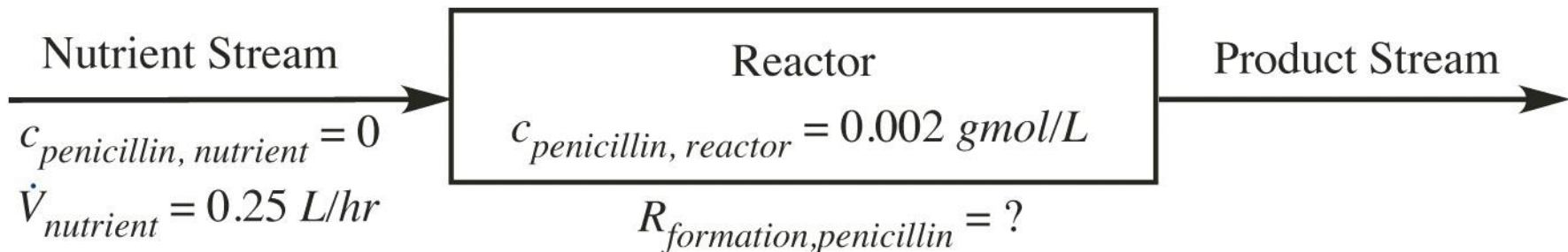


Example 5.4

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Material balances with formation or consumption where chemical reaction stoichiometry is not given

Ex. 5.5. Penicillin is produced in reactors containing the bacteria of the species *Penicillium chrysogenum*. A nutrient stream (containing no penicillin) is fed to a 10L reactor containing the bacteria. A product stream containing penicillin leaves the reactor (the bacteria stays in the reactor, and the penicillin concentration in the product stream is the same as inside the reactor). The densities of the nutrient and product stream can be assumed to be equal. What is the production rate of penicillin? The molecular weight of penicillin is 334.4.

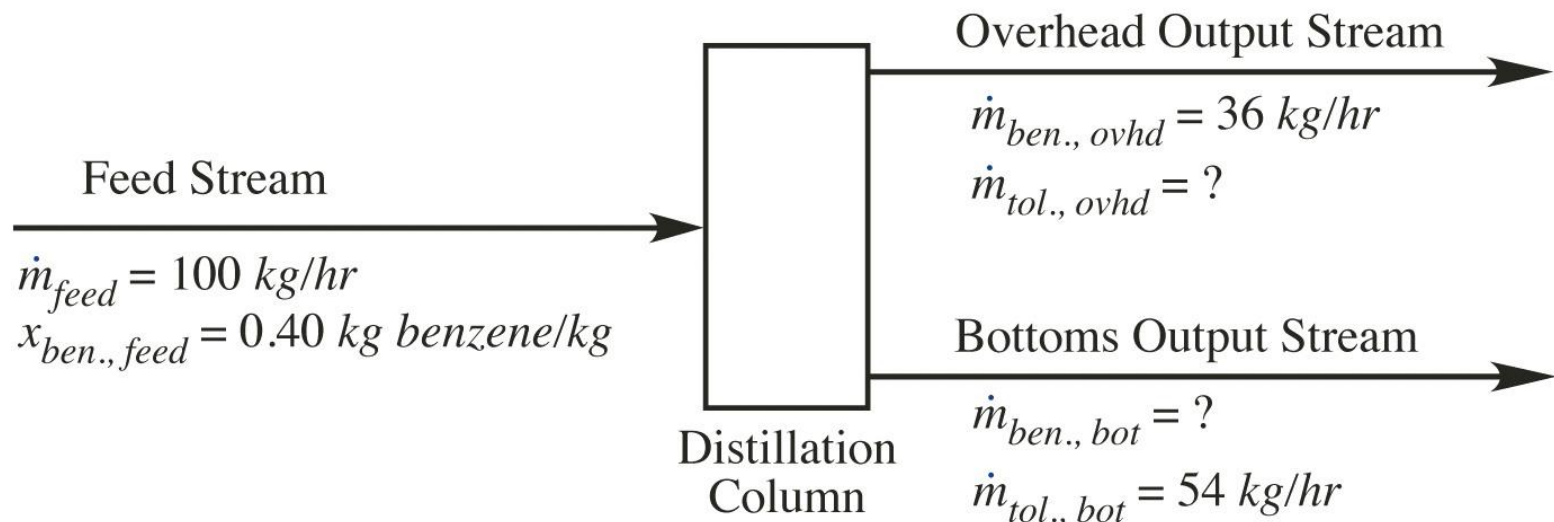


Example 5.5

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Material balances with no formation or consumption

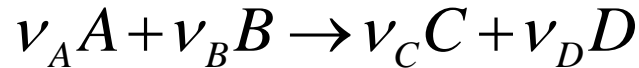
Ex. 5.6. Benzene and toluene are partially separated using a distillation column. The feed stream of 100kg/hr contains benzene at a mass fraction of 0.4, with the balance being toluene. In the overhead output stream, the benzene flow rate is 36kg/hr, and in the bottoms output stream, the toluene flow rate is 54kg/hr. What are the toluene flow rate in the overhead output stream, and the benzene flow rate in the bottoms output stream?



Material balances with formation/consumption where chemical reaction stoichiometry is given

More convenient to use mole balances

$$\sum_{\substack{\text{input} \\ \text{streams}}} \dot{n}_{A,in} + r_{\text{formation},A} = \sum_{\substack{\text{output} \\ \text{streams}}} \dot{n}_{A,out} + r_{\text{consumption},A}$$

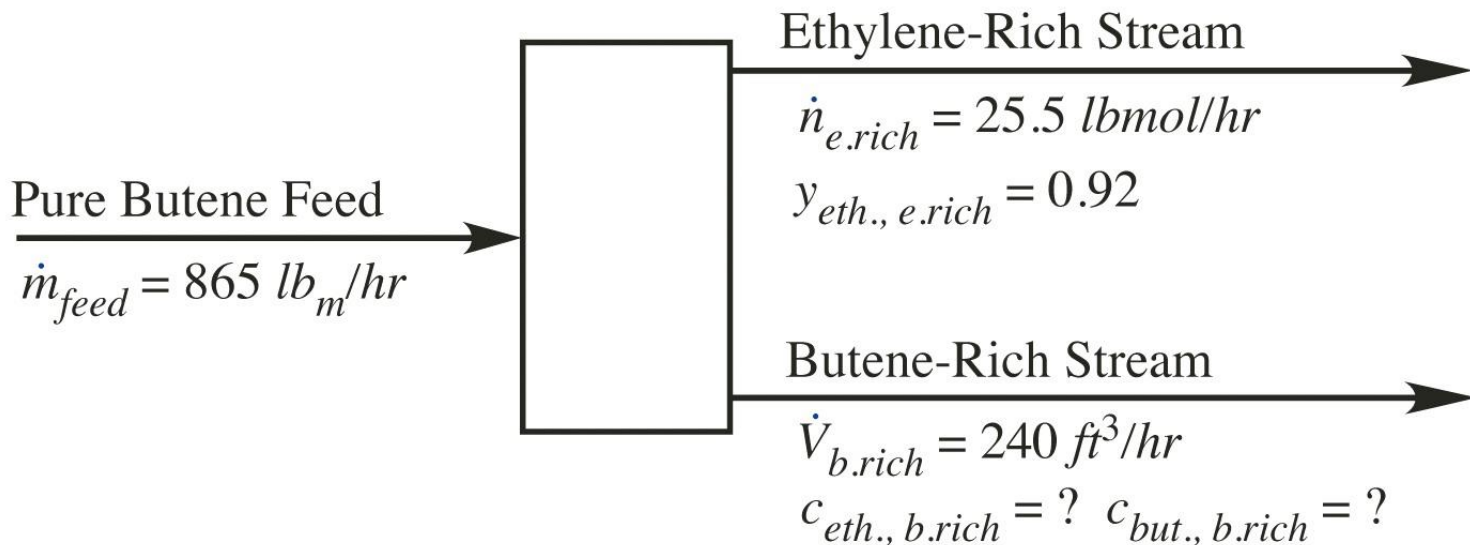
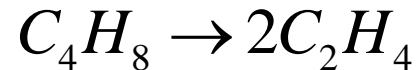


$$\frac{r_{\text{consumption},B}}{r_{\text{consumption},A}} = \frac{\nu_B}{\nu_A}, \quad \frac{r_{\text{formation},C}}{r_{\text{consumption},A}} = \frac{\nu_C}{\nu_A}, \quad \frac{r_{\text{formation},D}}{r_{\text{consumption},A}} = \frac{\nu_D}{\nu_A}$$

$$r_{\text{consumption},A} = X_A \sum_{\substack{\text{all input} \\ \text{streams}}} \dot{n}_{A,in}$$

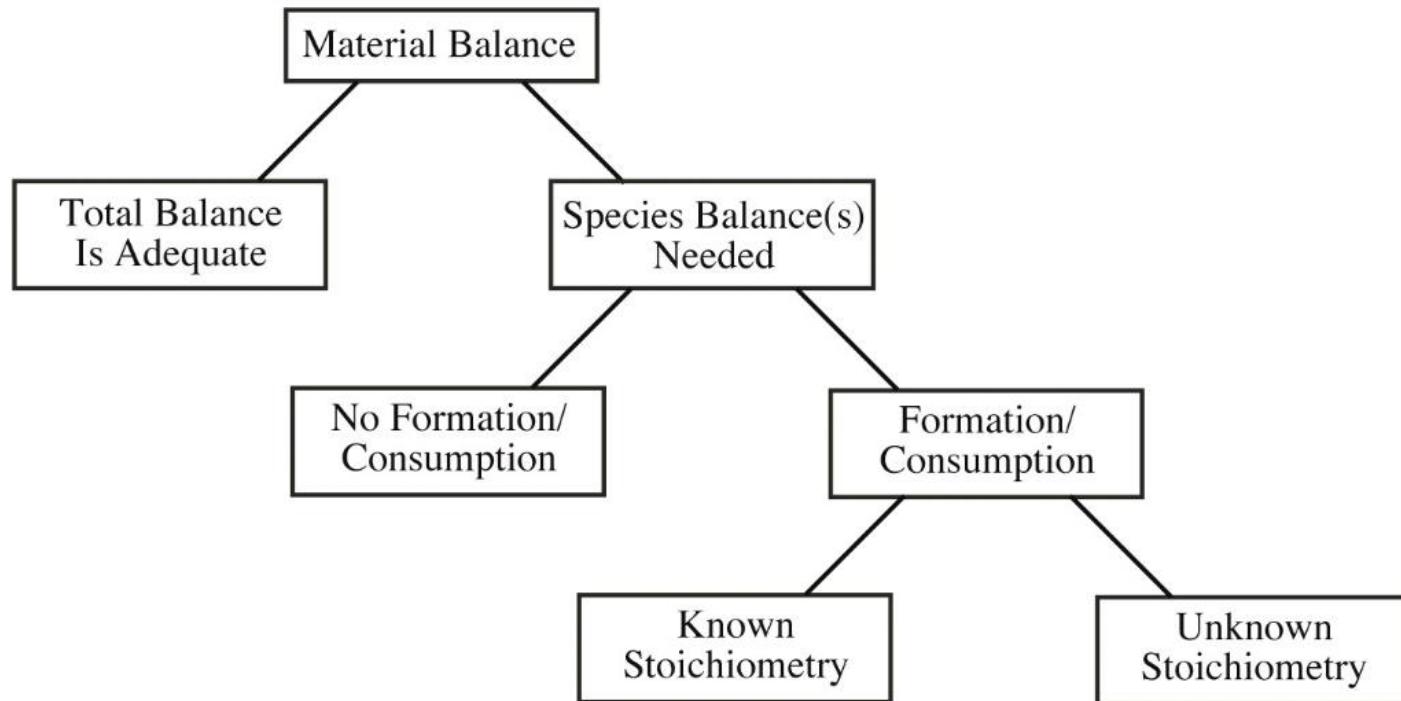
X_A : fractional conversion of A

Ex. 5.7. You are designing a process to convert excess butane to ethylene using the reaction. Of the incoming butane, 84% is converted to ethylene. What will be the concentrations of ethylene and butane in the butane-rich outlet stream?



Example 5.7

Decision-tree diagram for solving material-balance problems



- Is species information required, or will a total balance suffice?
- If species information is required, are there formation/consumption terms?
- If there are formation/consumption terms, is the reaction stoichiometry known or unknown?