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Engineering Innovation
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Chemical Engineering

Chemical Engineering!

Chemists vs. Chemical Engineers

What is Chem Eng and Why do We Care?

Transport Phenomena

Mass and Energy Balances

Separations (Distillation and Chromatography)

Chemist **vs.** Chemical Engineer

Chemist > test tube.

http://www.careersinoilandgas.com/build-your-career/working-in-oil-gas/career-options/engineers/chemical-engineers.aspx#.VCwU5PldXl8

Chemical engineer > 10,000 liter, continuous process reactor at a rate of 1000 liters/second.

Chemist **vs.** Chemical Engineer

Chemists determine reactions to make new compounds in a test tube

Chemical Engineers design processes to make compounds at a rate of 1000 L/min that are efficient and don't explode.

Chemical Engineers have backgrounds in chemistry AND fluid dynamics, heat transfer, materials science, thermodynamics …

June 4, 2012
CEN

CHEMISTS VS. CHEMICAL ENGINEERS

Chemical engineering grads were less likely to pursue further study and tended to be more highly paid than chemists

	B.A./B.S.		M.S.		PH.D.	
	CHEMISTS	CHEMICAL ENGINEERS	CHEMISTS	CHEMICAL ENGINEERS	CHEMISTS	CHEMICAL ENGINEERS
BY EMPLOYMENT						
Full-time	31%	52%	50%	43%	32%	61%
Part-time	9	6	7	5	4	2
Further study	43	25	23	19	51	28
Unemployed	17	17	21	33	12	9
Seeking	14	13	18	19	9	9
Not seeking	4	4	3	14	3	0
BY EMPLOYER						
Academia	44	25	43	29	60	14
Industry	47	72	54	71	29	66
Government	8	2	3	0	12	20
Self-employed	1	1	0	0	0	0
BY GENDER						
Women	55	41	54	14	42	36
BY CITIZENSHIP						
Non-U.S. resident	2	1	8	48	21	18
SALARIES ($ thousands)						
Full-time permanent	$36.0	$65.0	$51.8	$77.0	$75.0	$92.8

NOTE: Median salary data for all responding 2011 graduates regardless of experience. Numbers may not add to 100% because of rounding.

http://cen.acs.org/articles/90/i23/Starting-Salaries.html

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Engineering is an outstanding salary.

	Field	Starting Salary
1	Petroleum Engineering	$98,000
2	Chemical Engineering	$67,500
3	Nuclear Engineering	$66,800
4	Electrical Engineering	$63,400
5	Computer Engineering	$62,700
6	Aerospace Engineering	$62,500
7	Mechanical Engineering	$60,100
7	Materials Science & Engineering	$60,100
8	Industrial Engineering	$59,900
9	Software Engineering	$59,100
10	Computer Science	$58,400
10	Electrical Engineering Technology	$58,400
11	Actuarial Mathematics	$56,100
12	Biomedical Engineering	$54,900
13	Civil Engineering	$53,800

2012-2013 PayScale College Salary Report

Social Work	$33,100
Liberal Arts	$35,300
Biology	$39,100
Chemistry	$44,700
Mathematics	$48,500

Johns Hopkins
Whiting School of Engineering

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Why do we care about Chemical Engineering?

Look around you – nearly everything you see has parts designed by chemical engineers!

Toothpaste

Paint

Dyes

Hydrogen

Fertilizer

Shampoo

Gasoline

Decaffeinated Coffee

Soap

Food additives

Cosmetics

Polymers

Pharmaceuticals

Sugar

Chemical engineering is also important to food and medicine …

Chemical engineering contributes to the fertilizer industry that helps enhance food production.

Chemical engineers developed synthetic rubber, penicillin, and plastics.

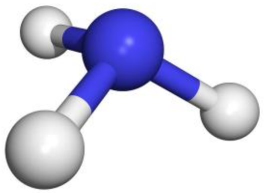
If that is not enough …

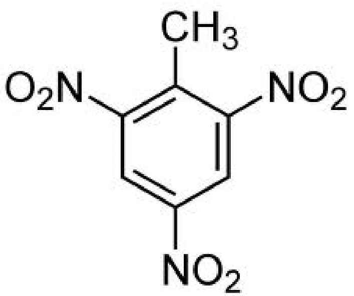
- In the United States
  - 170 Major Chemical Companies
  - $400 Billion a year
  - Employs more than a million workers

What Kind of Molecules do Chemical Engineers Work With?

Small and Simple

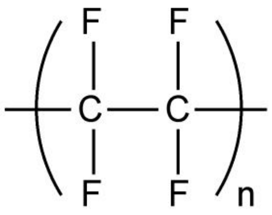
- Helium, He
- Ammonia, NH_3
- Hydrogen Fluoride, HF
- Trinitrotoluene, $C_6H_2(NO_2)_3CH_3$





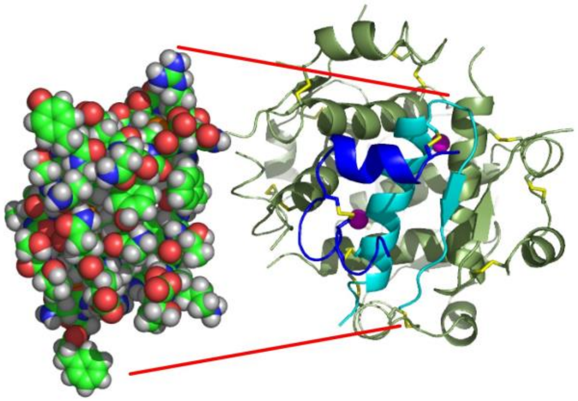
Large and Simple

- Polytetrafluoroethylene (teflon)



Large and Complicated

- Insulin, $C_{257}H_{383}N_{65}O_{77}S_6$



How are Chemicals Produced?

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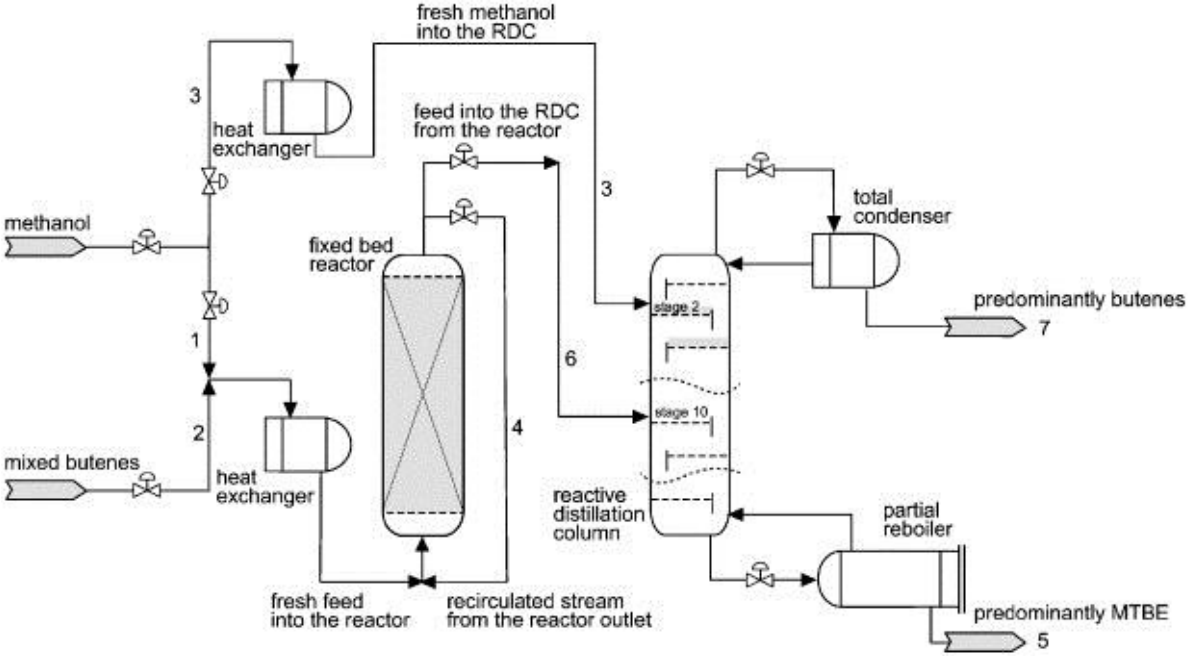
Reactions: Create new molecules out of two or more constituent components in a reactor.



Separations: Attempt to isolate a substance that is contained in a mixture of other ingredients

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Chemical Engineers need to understand:

Transport (flow and mixing of molecules)

Thermodynamics (energy and heat)

Material and Energy Balances (conservation laws)

Chemical Production in Reactors

Raw materials →

Catalyst →

Energy →

→ *Product*

→ *Byproducts*

→ *Raw materials*

→ *Catalyst*

→ *Energy*

Chemical Production in Reactors

Raw materials →

Catalyst →

Energy →

→ *Product*

→ *Byproducts*

→ *Raw materials*

→ *Catalyst*

→ *Energy*

Exothermic Reactions

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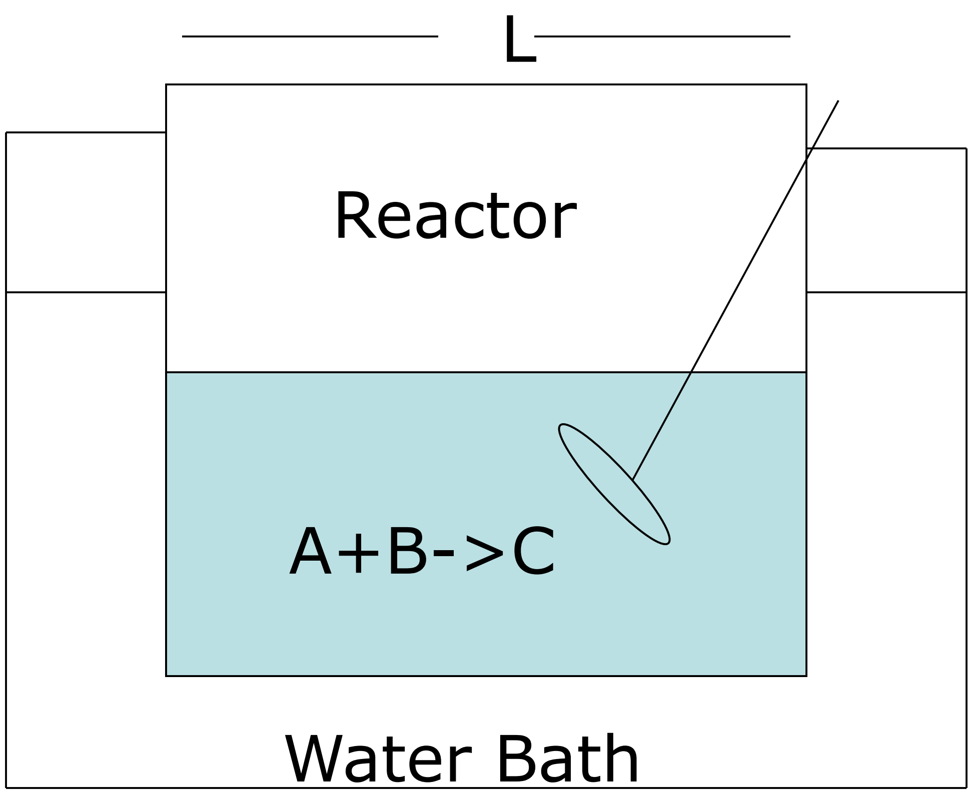

Energy Produced by reaction is proportional to reactor volume (L^3)

Energy Removed is proportional to surface area (L^2)

Possible Scale up Problem

Efficient Engineering

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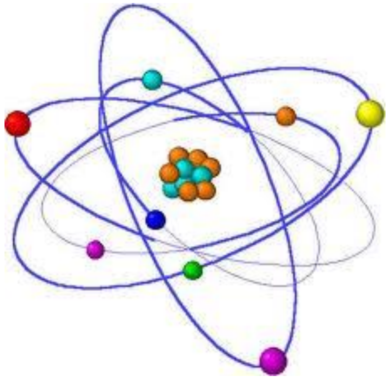
H_2SO_4 (Sulfuric Acid)

40 million tons per year in US

Almost 250 million tons per year worldwide

There is a significant impact if you are able to improve the efficiency of the process by 1% (better mixing, improved reactor design, etc.)

Quantities in a Chemical Reaction



- Grams
- Atoms
- Moles
  - a chemical mass unit, defined to be 6.022 x 10^{23} molecules, atoms, or some other unit
  - mass of a mole is the gram formula mass of a substance

How big is a mole?

If you were given a mole of dollars when you were born, how many years would it take to spend all your money if you spent:

$1 million dollars every day?

$1 million dollars every hour?

$1 million dollars every second?

Periodic Table of the Elements

1 H 1.00794																1 H 1.00794	2 He 4.002602
3 Li 6.941	4 Be 9.012182											5 B 10.811	6 C 12.0107	7 N 14.00674	8 O 15.9994	9 F 18.9984032	10 Ne 20.1797
11 Na 22.989770	12 Mg 24.3050											13 Al 26.981538	14 Si 28.0855	15 P 30.973761	16 S 32.066	17 Cl 35.4527	18 Ar 39.948
19 K 39.0983	20 Ca 40.078	21 Sc 44.955910	22 Ti 47.867	23 V 50.9415	24 Cr 51.9961	25 Mn 54.938049	26 Fe 55.845	27 Co 58.933200	28 Ni 58.6934	29 Cu 63.546	30 Zn 65.39	31 Ga 69.723	32 Ge 72.61	33 As 74.92160	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.4678	38 Sr 87.62	39 Y 88.90585	40 Zr 91.224	41 Nb 92.90638	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.90550	46 Pd 106.42	47 Ag 107.8682	48 Cd 112.411	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.90447	54 Xe 131.29
55 Cs 132.90545	56 Ba 137.327	57 La 138.9055	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.23	77 Ir 192.217	78 Pt 195.078	79 Au 196.96655	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.98038	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (266)	110 (269)	111 (272)	112 (277)		114 (289) (287)		116 (289)		118 (293)

58 Ce 140.116	59 Pr 140.90765	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.964	64 Gd 157.25	65 Tb 158.92534	66 Dy 162.50	67 Ho 164.93032	68 Er 167.26	69 Tm 168.93421	70 Yb 173.04	71 Lu 174.967
90 Th 232.0381	91 Pa 231.03588	92 U 238.0289	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

S.E. Van Bramer, 7/22/99

1995 IUPAC masses and Approved Names from http://www.chem.qmw.ac.uk/iupac/AtWt/

masses for 107-111 from C&EN, March 13, 1995, P 35

112 from http://www.gsi.de/z112e.html

114 from C&EN July 19, 1999

116 and 118 from http://www.lbl.gov/Science-Articles/Archive/elements-116-118.html

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Cool Periodic Table Websites

The University of Kentucky's Comic Book Periodic Table

http://www.uky.edu/Projects/Chemcomics/

The Los Alamos National Lab Periodic Table

http://periodic.lanl.gov/index.shtml

Molar Mass

Calculate the molar mass of methane, CH_4.

How many moles of methane are found in 25kg of methane?

How many molecules of methane are found in 25kg of methane?

If a solution has 25 grams of water and 25 grams of methanol, CH_3OH, what is the mole fraction of ethanol in the solution?

Take a break?

What do these processes have in common?

- Hydrogen embrittlement of pressure vessels in nuclear power plants?
- Flow of electrons through conductors
- Dispersion of pollutants from smoke stacks
- Transdermal drug delivery
- Influenza epidemics
- Chemical reactions
- Absorption of oxygen into the bloodstream

They all depend on DIFFUSION (Conduction)

- What is diffusion? The transport of material –atoms or molecules – by random motion
- What is conduction? The transport of heat or electrons by random motion

What happens when you place a drop of ink into a glass of water?

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Brownian motion causes the ink particles to move erratically in all directions.

Why does random motion cause spreading of a concentration of particles?

Because there are more ways for the particles to drive apart than there are for the particles to drift closer together.

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Transport Phenomena

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Moving of a property from one place to another down a gradient

- Flow of electrons through conductors
- Transdermal drug delivery
- Influenza epidemics

Three types of Transport Phenomena

- **Momentum Transfer**
  - Transfer of momentum across/down a gradient
- **Heat Transfer**
  - Heat is moved by transfer of energy down a gradient
- **Mass Transfer**
  - Material moved by diffusion down a gradient

All are proportional to a flux (rate of flow per area)

Consider a cup of coffee

Momentum Transfer: Stir with a spoon; all molecules (even if not in contact with the spoon) will move

Heat Transfer: Add creamer, the creamer and coffee eventually reach the same temperature

Mass Transfer: Add creamer; the creamer and coffee do not stay separated

Momentum Transfer

Liquid moved by transfer of velocity down a gradient (fast →slow)

Newton's Law:

$$\tau_{zx} = -\mu \frac{dv_x}{dz}$$

τ_{zx} = momentum flux = $(\frac{mass}{length*time^2})$

μ = viscosity = $(\frac{mass}{length*time})$ [gases ~ 0.001$\frac{gram}{cm*s}$; liquids ~1 $\frac{gram}{cm*s}$]

$\frac{dv_x}{dz}$= velocity gradient = $\frac{1}{time}$

Heat Transfer

Heat transfer occurs by three means:

Conduction

Convection

Radiation

Heat Transfer

Heat moved by transfer of energy down a gradient (hot → cold)

Fourier's Law (conduction):

$$q_z = -k\,\frac{dT}{dz}$$

q_z = heat flux = $\frac{energy}{length^2 * time}$

k = thermal conductivity = $\frac{energy}{length * time * temperature}$

[gases~0.0001$\frac{cal}{cm*s*°C}$; $liquids$~0.001 $\frac{cal}{cm*s*°C}$; $solids \sim 0.1\,\frac{cal}{cm*s*°C}$]

$\frac{dT}{dz}$ = Temperature gradient = $\frac{Temperature}{length}$

Mass Transfer

Material moved by diffusion down a gradient (high→ low conc.)

Fick's Law:

$$J_i = -D\frac{dc_i}{dz}$$

J_i = mass flux = $\frac{mass}{length^2 * time}$

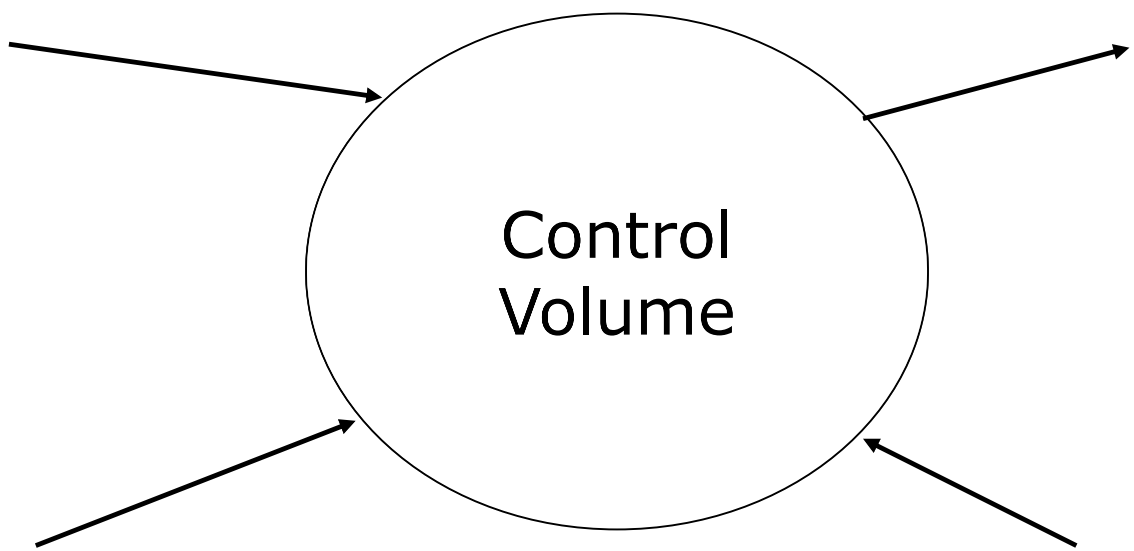
D = Diffusivity = $\frac{length^2}{time}$

[gases~0.1$\frac{cm^2}{s}$; liquids~0.00001$\frac{cm^2}{s}$; solids~0.000000001$\frac{cm^2}{s}$]

$\frac{dc_i}{dz}$ = Concentration gradient = $\frac{mass}{length^4}$

Mass and Energy Balances

Input + Generation – Output - Consumption = Accumulation



For non-reacting system,
Generation = ?

For non-reaction system,
Consumption = ?

For systems operating
at steady-state,
Accumulation =?

chemical processes

IV. Mass and energy balance

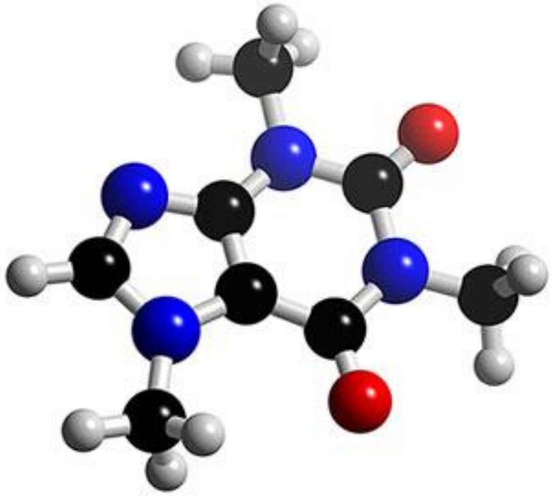
$$In = Out \begin{cases} Total\ Balance: N_1 + N_2 = N_3 \\ A\ Balance: x_{1,A}N_1 + x_{2,A}N_2 = x_{3,A}N_3 \\ B\ Balance: x_{1,B}N_1 + x_{2,B}N_2 = x_{3,B}N_3 \\ C\ Balance: x_{1,C}N_1 + x_{2,C}N_2 = x_{3,C}N_3 \end{cases}$$

$$x_{A,1} + x_{B,1} + x_{C,1} = 1$$

4 independent equations, therefore can solve for 4 unknowns!

Why do we do separations?

- Acquire something useful ($)
- Remove something harmful [-(-$)]



Caffeine

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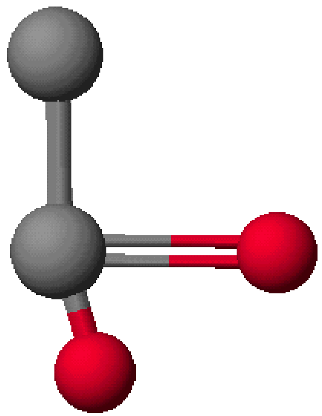
How would you separate these coins?

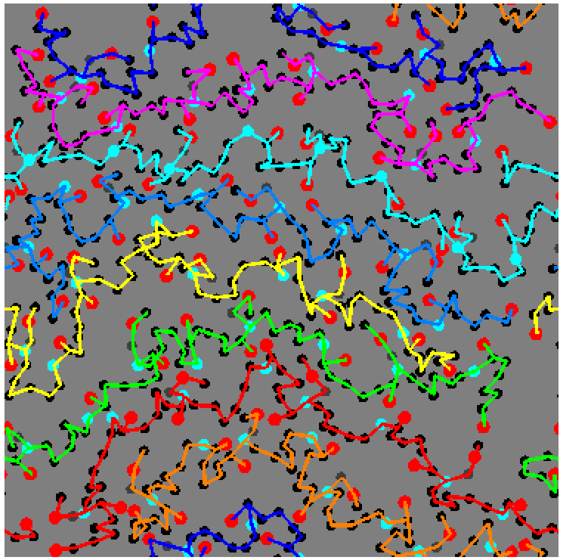
How do you separate things?



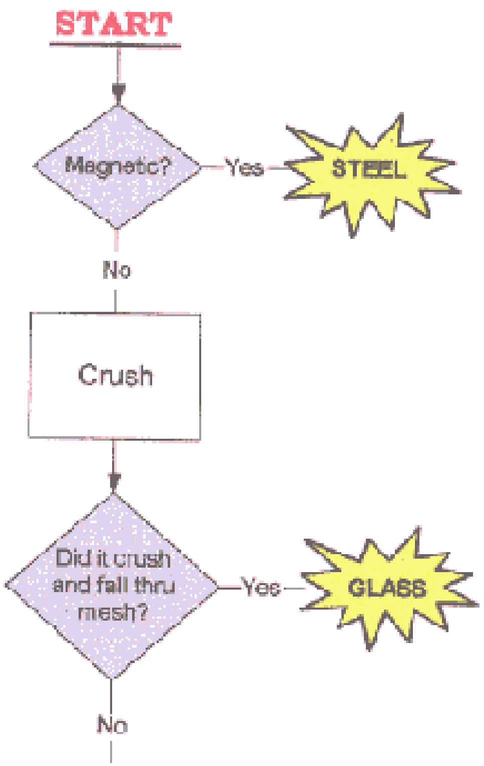
Based on their differences.

Properties of a Single Substance

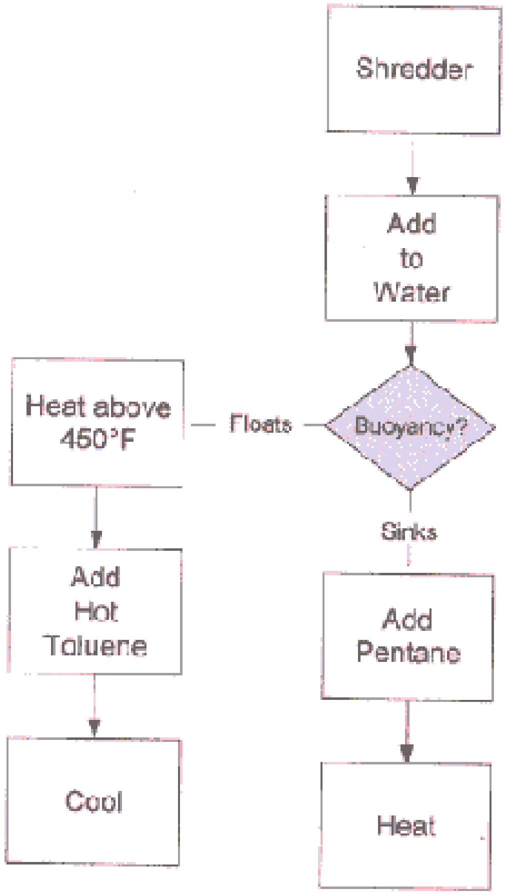
- Boiling Point
- Freezing Point
- Density
- Volatility
- Surface Tension
- Viscosity
- Molecular Complexity
  - Size
  - Geometry
  - Polarization



Separations: Garbage



Garbage separation (cont.)



Garbage separation (cont.)

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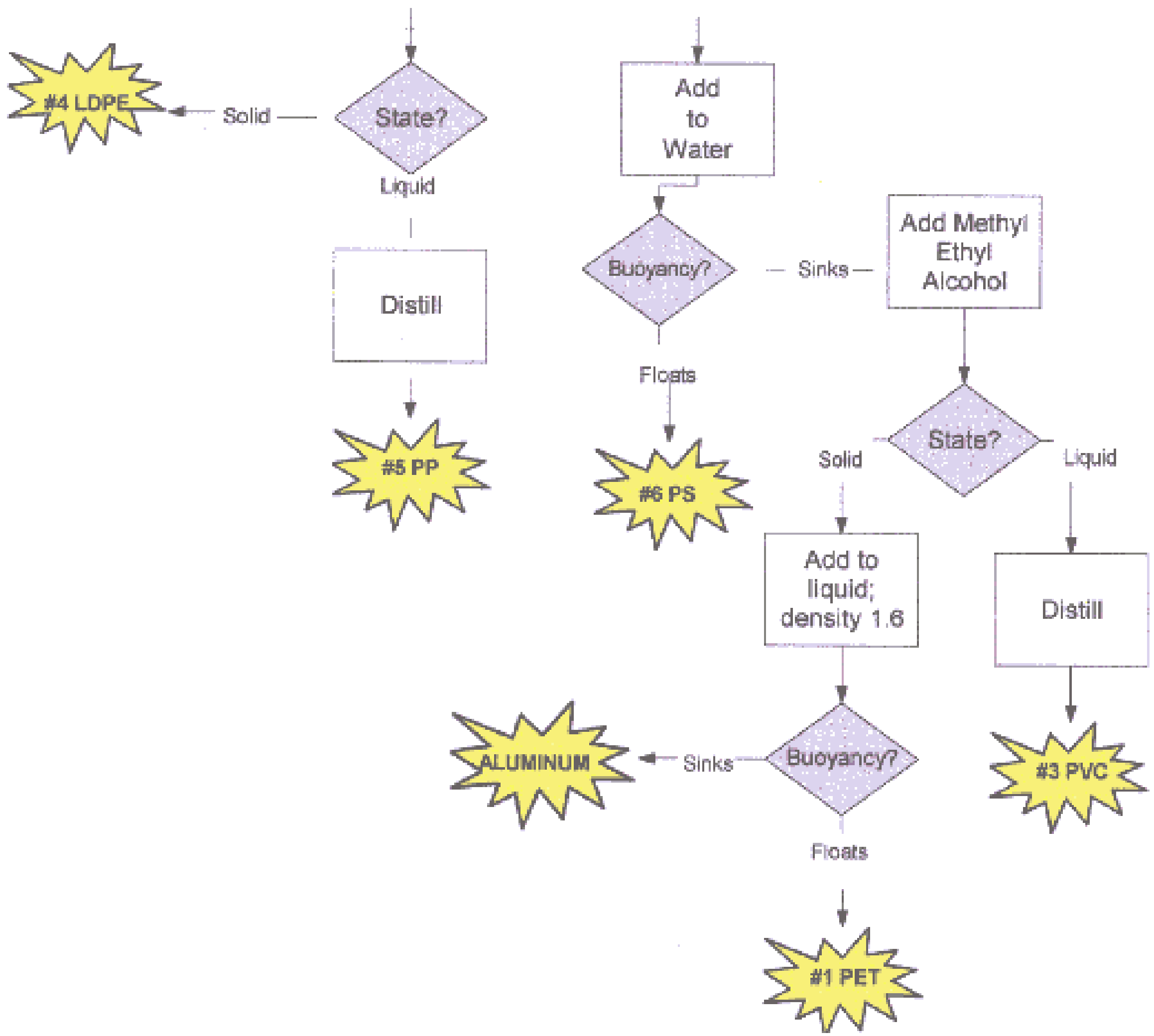


Separations: Unit Operations

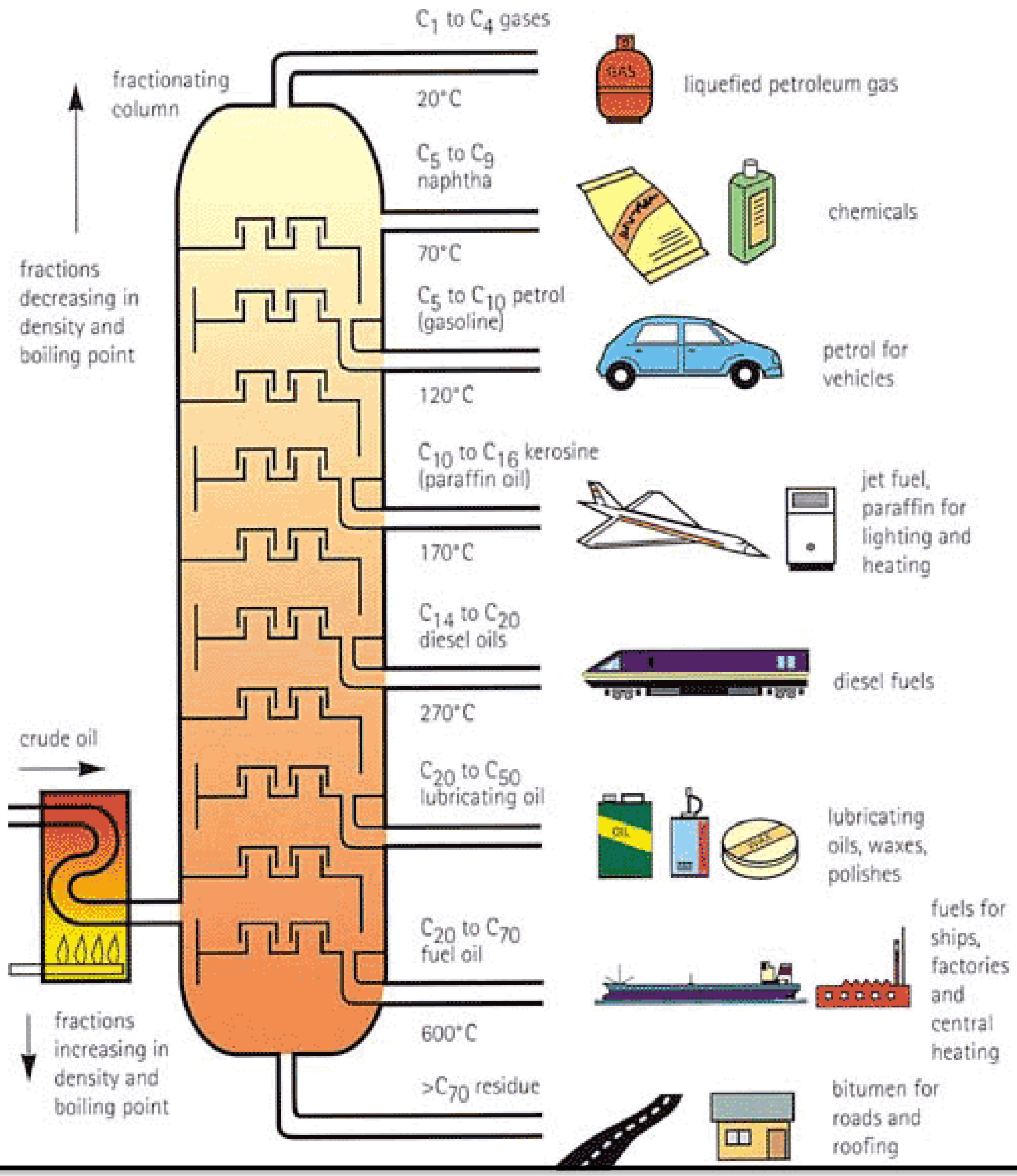
Use separation processes to:

- Purify raw materials
- Purify products
- Purify and separate unreacted feed.

Most common types:

- Distillation
  - Flash distillation
  - Batch distillation
  - Column distillation
- Extraction
- Absorption
- Stripping
- Chromatography

Refinery Distillation



http://ffden-2.phys.uaf.edu/212_spring2011.web.dir/kristine_odom/temp/10956/ftddrops/Downstream.html

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Chemical Distillation Lab

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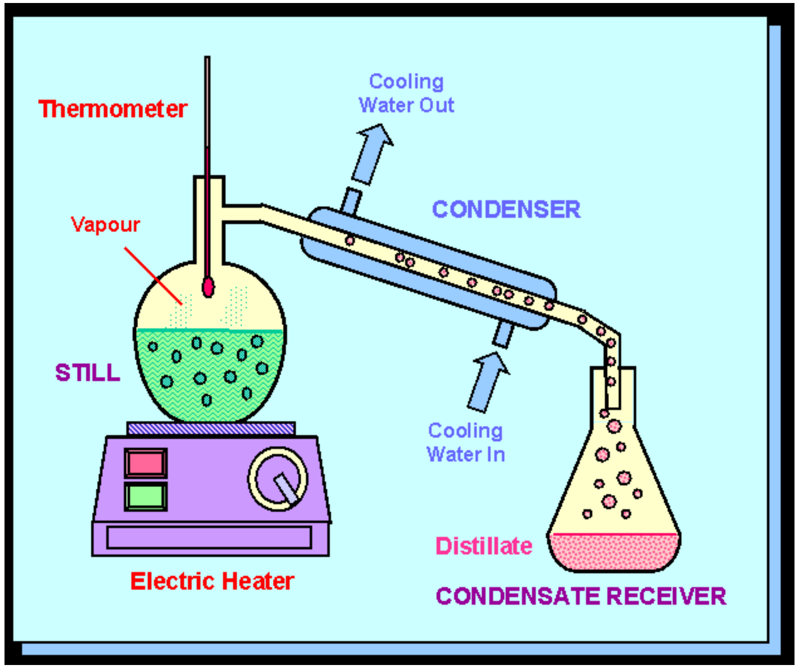
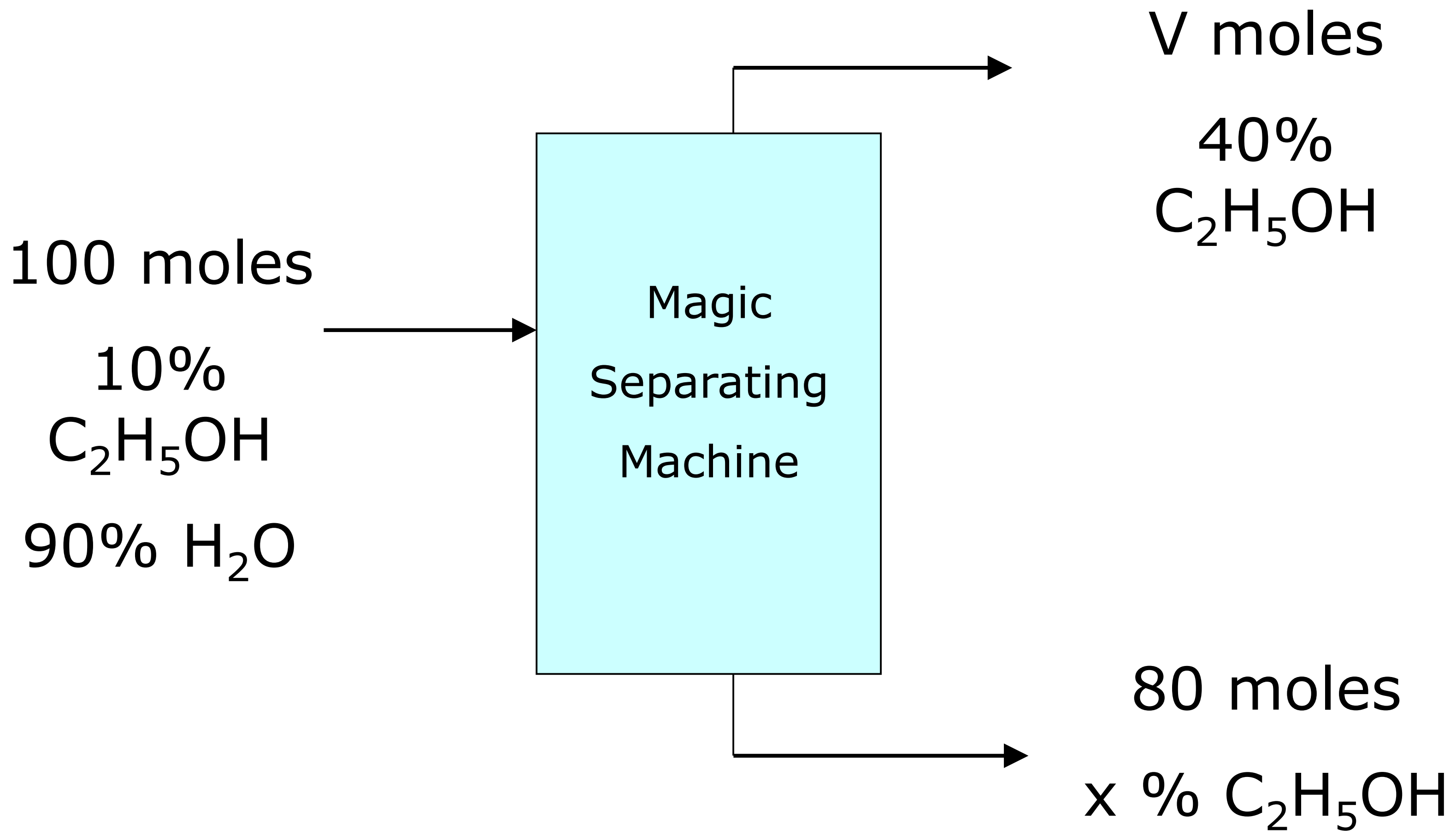


Boiling points

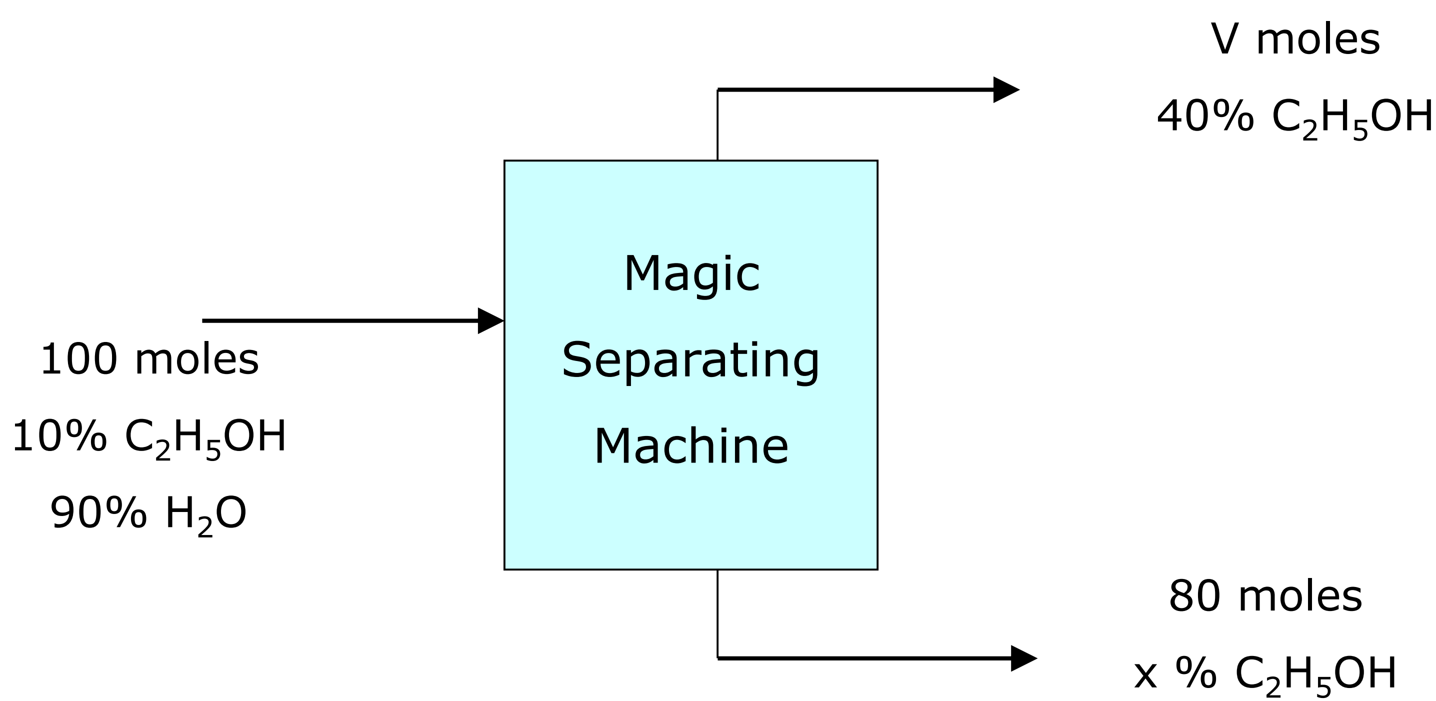
Ethanol = 78.4°C

Water = 100°C

Separations Calculation



Separations Calculation



Conservation of total Moles $100 - (V+80) = 0$; $V = 20$

Conservation of moles of C_2H_5OH $100*.1 - (.4*V + x*80) = 0$

$x = 2.5\%$

Equilibrium (Vapor-Liquid)

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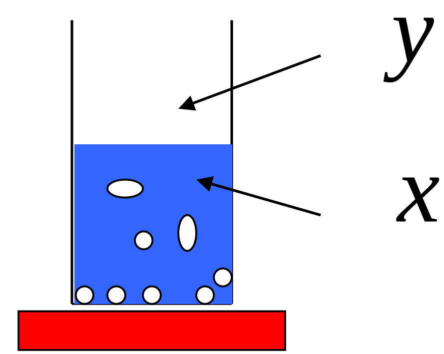
Consider an ethanol-water solution at its boiling point

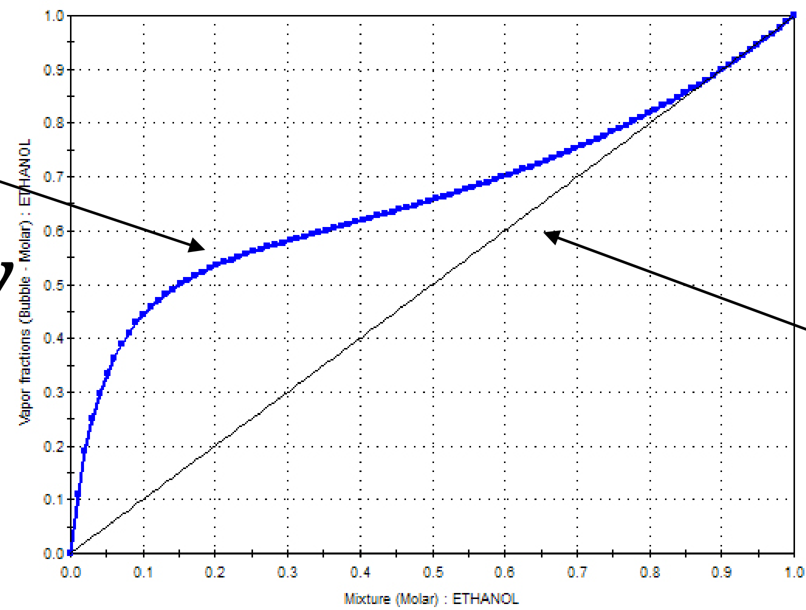
$y \equiv$ mole fraction ethanol in vapor

$x \equiv$ mole fraction ethanol in liquid



equilibrium curve

y



x

45° line
$(y = x)$

Simple Distillation

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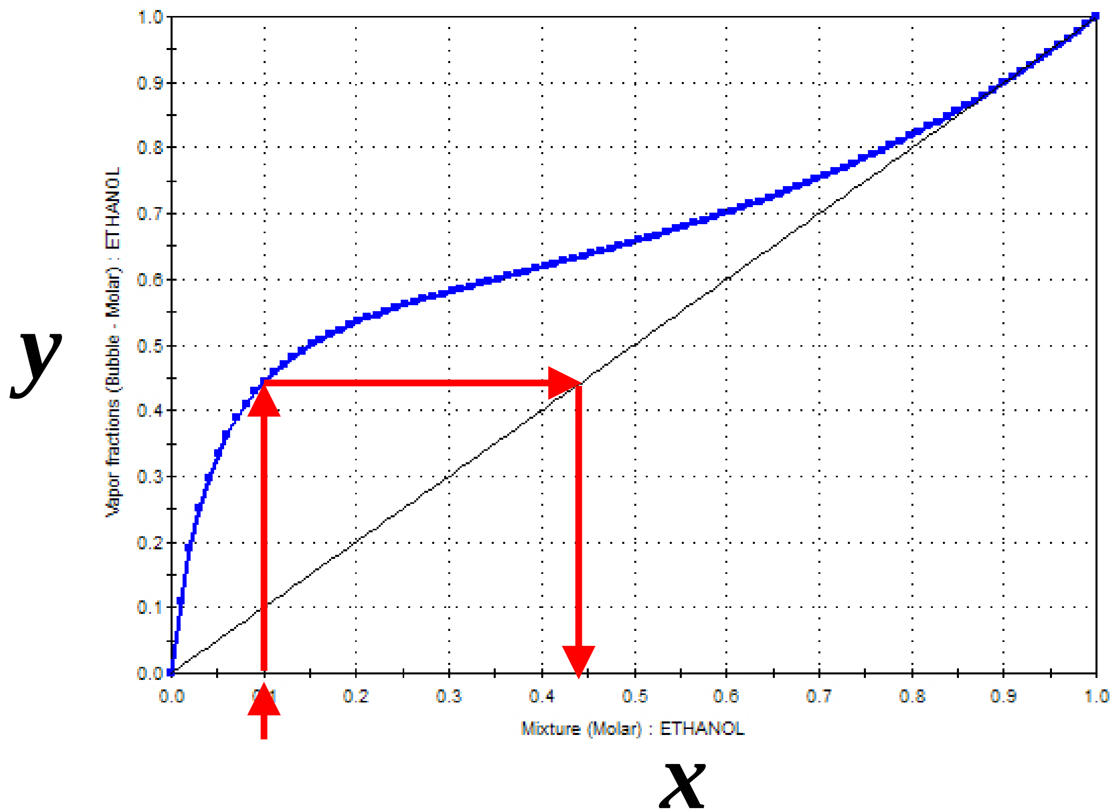

Start with 10-mol% ethanol solution (liquid).

Vapor is enriched to nearly 45-mol% ethanol.

Condense the vapor to collect the concentrated ethanol.

How to get purer ethanol?

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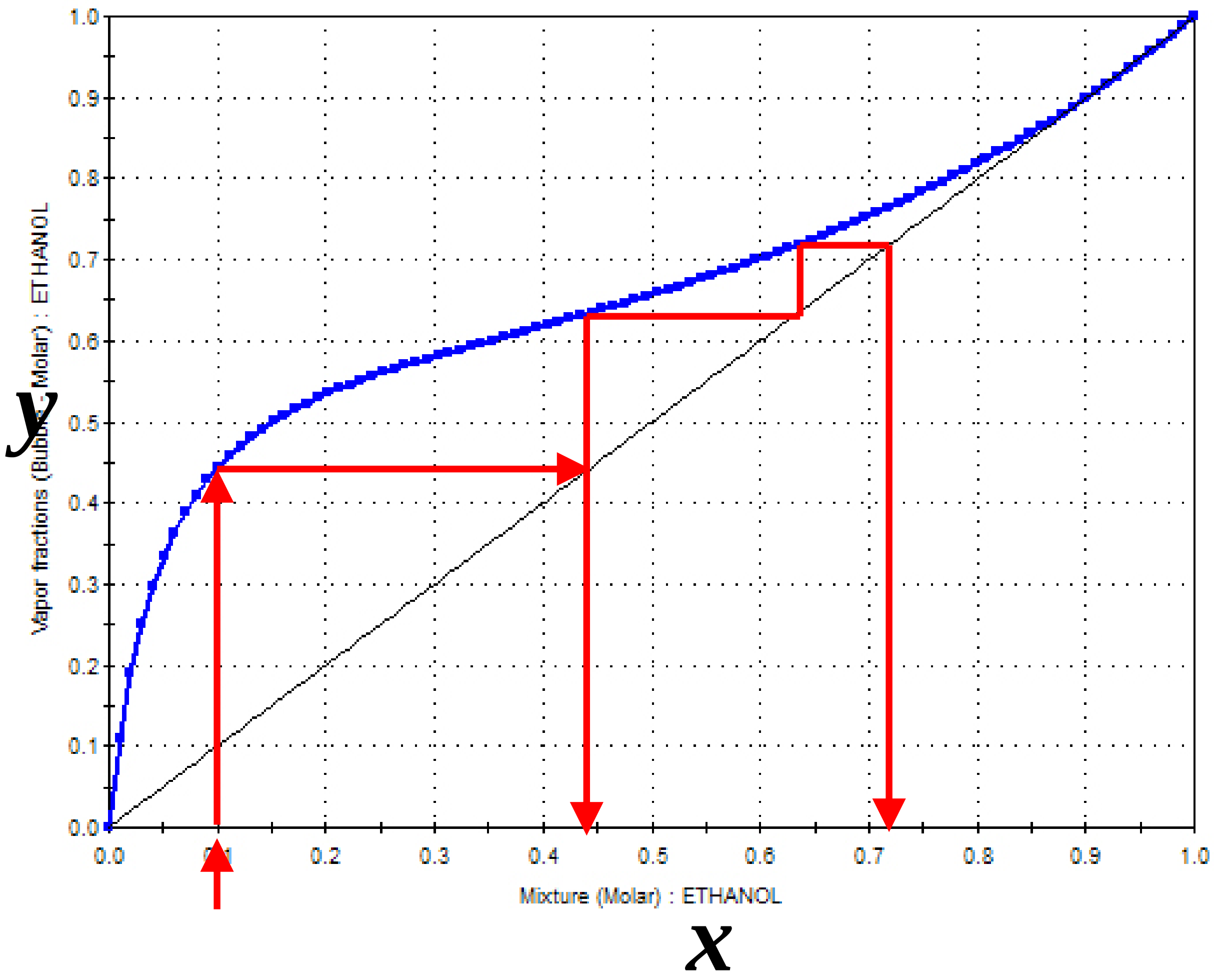

Azeotrope: 95.6% ethanol and 4.4% water

Redistill -- increase the number of stages.

Another Azeotrope

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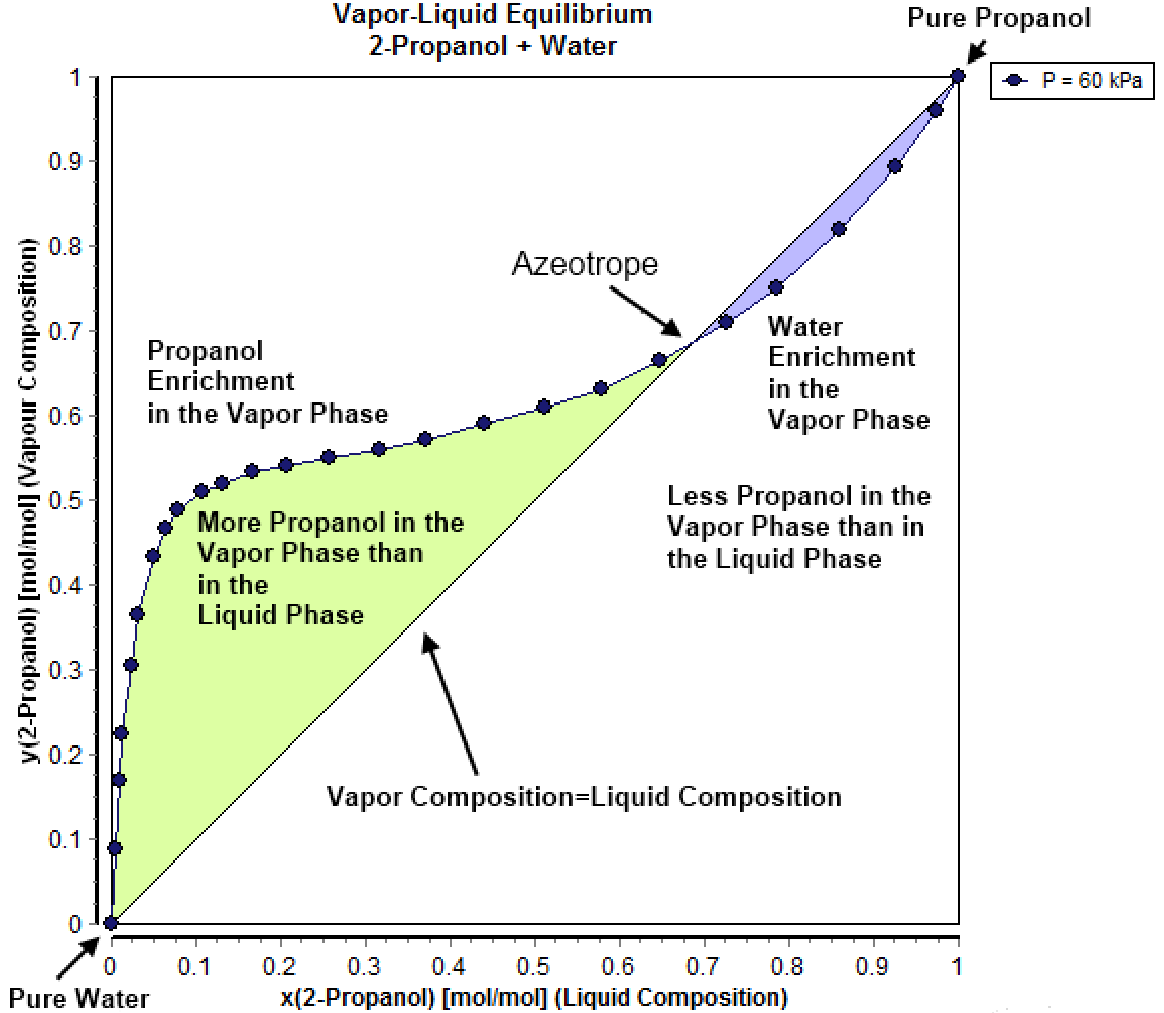

Data taken from Dortmund Data Bank
Original Source: Marzal P., Monton J.B., Rodrigo M.A., J.Chem.Eng.Data,:41(3), 608-611, 1996

How many stages would you need to go from 10 mole% 2-propanol to 60 mole%?

Take a break?

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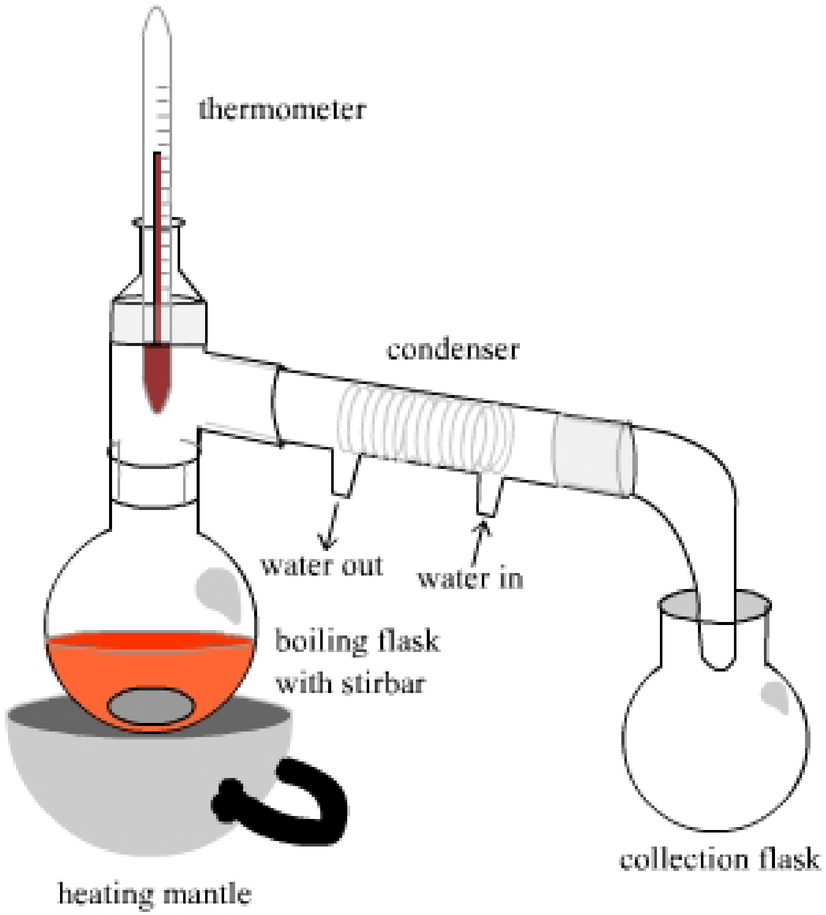
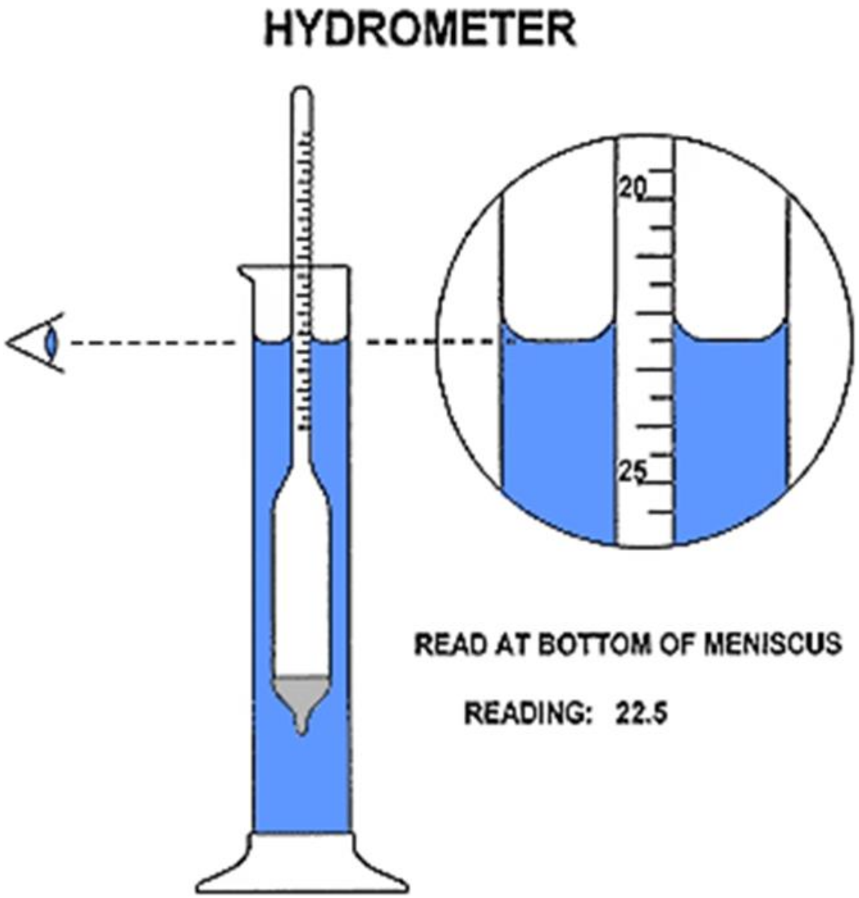


- Measure the temperature.
  - b.p. Ethanol = 78.4˚C
  - b.p. Water = 100˚C
- Measure the initial volume.
- Collect three samples.
- Measure
  - Temperature
  - Volume
  - Specific gravity.

How to measure specific gravity

- Hydrometer



Distillation

Use the temperature data and the specific gravity data to determine the weight percent ethanol in each sample.

Distillate #1

$T = 24.0\ ^{o}C$

s.g. = 0.920

From the Data Table

- At 20ºC

45% ethanol has specific gravity = 0.92472

46% ethanol has specific gravity = 0.92257

Distillate #1
T = 24.0 º C
s.g. = 0.920

At 25ºC

45% ethanol has specific gravity = 0.92085

46% ethanol has specific gravity = 0.91868

From the Data Table

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Interpolate between 20ºC and 25ºC to get the specific gravity of 45% ethanol at 24ºC.

$$sg_{45\%@24C} = 0.92472 - (24\text{-}20)*\left(\frac{0.92472-0.92085}{25-20}\right)$$

$$sg_{45\%@24C} = 0.92162$$

Interpolate between 20ºC and 25ºC to get the specific gravity of 46% ethanol at 24ºC.

$$sg_{46\%@24C} = 0.92257 - (24\text{-}20)*\left(\frac{0.92257-0.91868}{25-20}\right)$$

$$sg_{46\%@24C} = 0.91946$$

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From the Data Table

Now interpolate between 45% and 46% to get the actual concentration of ethanol.

Our sample has a specific gravity of 0.920 @ 24°C

$$\%\text{e-oh} = 46 + (0.91946-0.920)*\left(\frac{46-45}{0.92162-0.91946}\right)$$

$$sg_{45\%@24C} = 45.75\%$$

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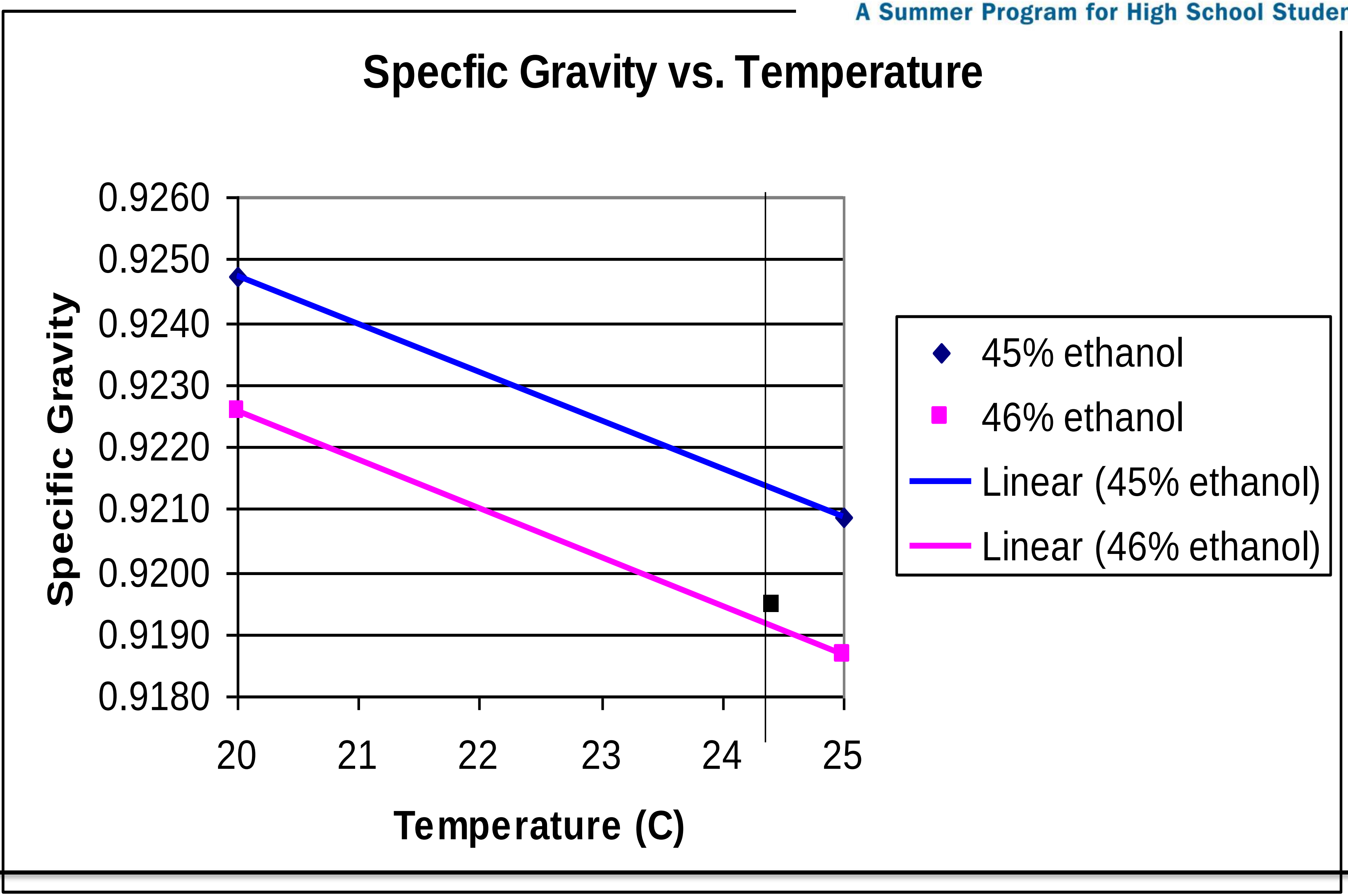
Specfic Gravity vs. Temperature
Specific Gravity
0.9260
0.9250
0.9240
0.9230
0.9220
0.9210
0.9200
0.9190
0.9180
20
21
22
23
24
25
Temperature (C)
45% ethanol
46% ethanol
Linear (45% ethanol)
Linear (46% ethanol)

Determine the % Ethanol in Distillate #1

At 24ºC the distance between the 45% and 46% alcohol lines is 1.2 cm.

At 24ºC the distance between the 45% and the data point is 0.9 cm.

- So
$$\frac{0.9}{1.2} = \frac{x}{1\%}$$
$$x = 0.75\%$$
- And the % ethanol = 45.75%

Grams of Ethanol in each solution

Mass of Distillate #1

= volume of the solution * specific gravity

Grams of ethanol in Distillate #1

= grams of solution * % alcohol ÷ 100

Moles of ethanol

= grams of ethanol ÷ 46.07 g/mol

Grams of Water in each Solution

Calculate the total moles of water in each sample

moles of H_2O= grams of H_2O ÷ 18.02grams/mole

Perform a mole balance analysis for ethanol and water to check whether all material is accounted for.

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Calculate the total electrical energy input for both experiments (with and without the lid):

$$\text{E(Joules)} = \text{average watts} \times \text{seconds}$$

Calculate the water's energy increase for both experiments:

$$\text{E(Joules)} = \text{water mass} \times \frac{4.186\,\text{J}}{\text{g}\ {}^{\text{o}}\text{C}} \times \left(\text{T}_{\text{f}} - \text{T}_{\text{i}}\right)$$

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Calculate the efficiencies with and without the lid:

$$e = \frac{\text{water's energy increase}}{\text{total electrical energy input}}$$

What difference did putting a lid on the pot make?

If the efficiency is less than 1.0, where did the remaining energy go? Try to think of all possible “losses”.

How could you improve the efficiencies?

Chromatography Lab

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- Mobile phase
- Stationary phase
- Paper Chromatography
- Solute-solvent interactions vs. solute-stationary phase interactions

Dye Flow Rates

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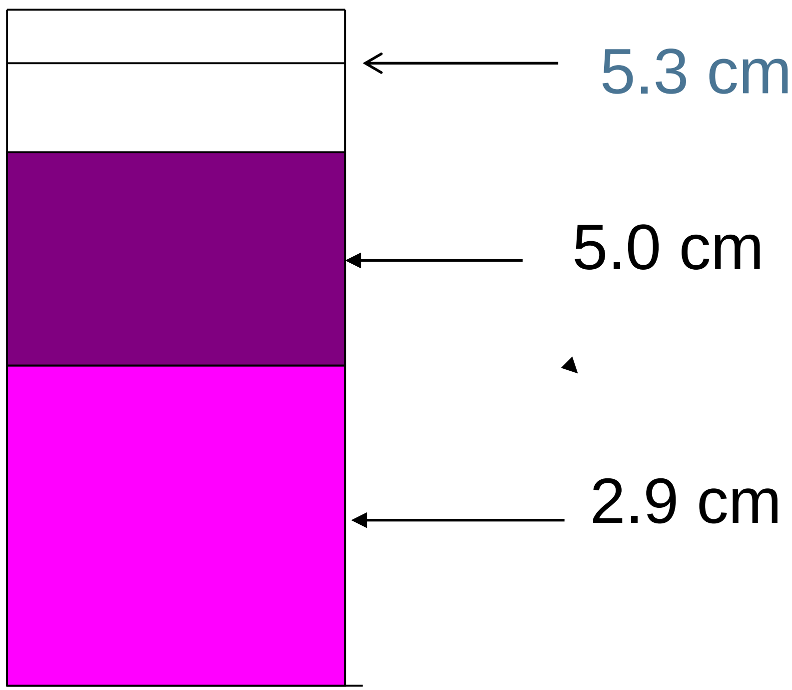

Flow rate of pink (retention factor) = 2.9/5.3 = 0.55

Flow rate of purple (retention factor) = 5.0/5.3 = 0.94

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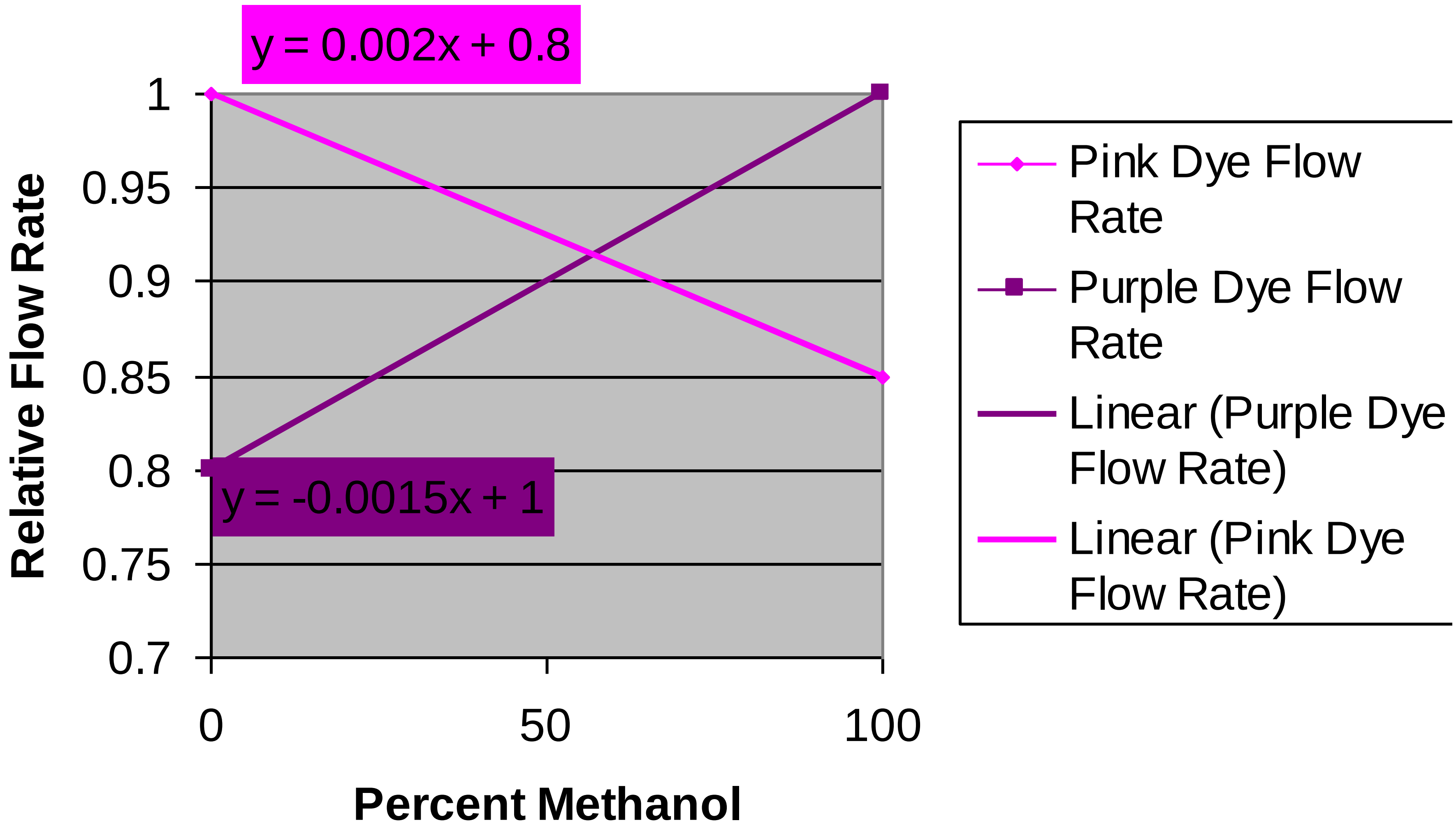
Dye Flow Rate vs. Percentage Methanol



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