Syllabus

Reaction Engineering I
(458.303.001)

Course Objectives

Students should be able to express basic concepts of reaction kinetics, chemical equilibria, design and evaluate operational performance of ideal, isothermal, adiabatic of batch and flow reactors for homogeneous reactions by using computer software package.

1. Provide a general understanding of the analysis and design chemical reactors.
2. Provide instruction in the analysis of experimental data to obtain rate equations.
3. Provide instruction in the formulation of reaction engineering design problems
4. Provide instruction in the solution using mathematical analysis & computer tools.
5. Provide instruction in the optimization of reactor/separator/recycle systems to achieve optimize profits .
6. Provide instruction in the safety consideration in reaction engineering problem
7. Provide instruction in the development of engineering judgment .

Course topics

- Types of reactors in practice, the three "ideal" reactors: batch, CSTR, plug flow
- Writing mole balance for single reaction in the three ideal reactor types
- Reaction rate law, reaction stoichiometry and their combination
- Comparison of performance characteristics of ideal reactor types
- Data collection and analysis to determine rate equations
- Reactors in series or in parallel
- Selection of reactor types in reactor design or lab. scale reactor for kinetics
- Variable fluid density and pressure drop in flow reactors
- Reactors combined with separators and recycle, optimization
- Multiple reactions, selectivity, yield, reactor selection, optimization

Office hours

Monday, Wednesday 12:15-15:00 pm @ 302-726
(For quick questions ask me after class.)

Course home page

http://sfpl.snu.ac.kr/

E-mail

The class is too big for e-mail to be reasonable.
Please use the office hours. E-mail will be ignored.

Grades Distribution

Attendance:	**5 %**
HW:	**15 %**
Quizzes :	**20 %**
Mid-term Ex.:	**20 %**
Final Ex:	**40 %**
	100 %

There will be **no** make-up exams and quizzes.

Grade Scale

A: 20-30%, B:30-40%, C or below 30-50%

Repeaters will be scaled separately follow the above scale

Lecture Schedule

1st week: Introduction, Mole Balance (Chap 1)

2rd week: Conversion and Reactor Sizing (Chap 2)

3rd - 4th week: Rate Law and Stoichiometry (Chap 3)

5th - 6th week: Isothermal Reactor Design (Chap 4)

7th-8th week: Collection and Analysis of Rate Data (Chap 5)

9-11th week: Multiple Reactions (Chap 6)

12th -15th week: Nonelementary Reaction Kinetics (Chap7)

Exam Schedule

Place: 302-409

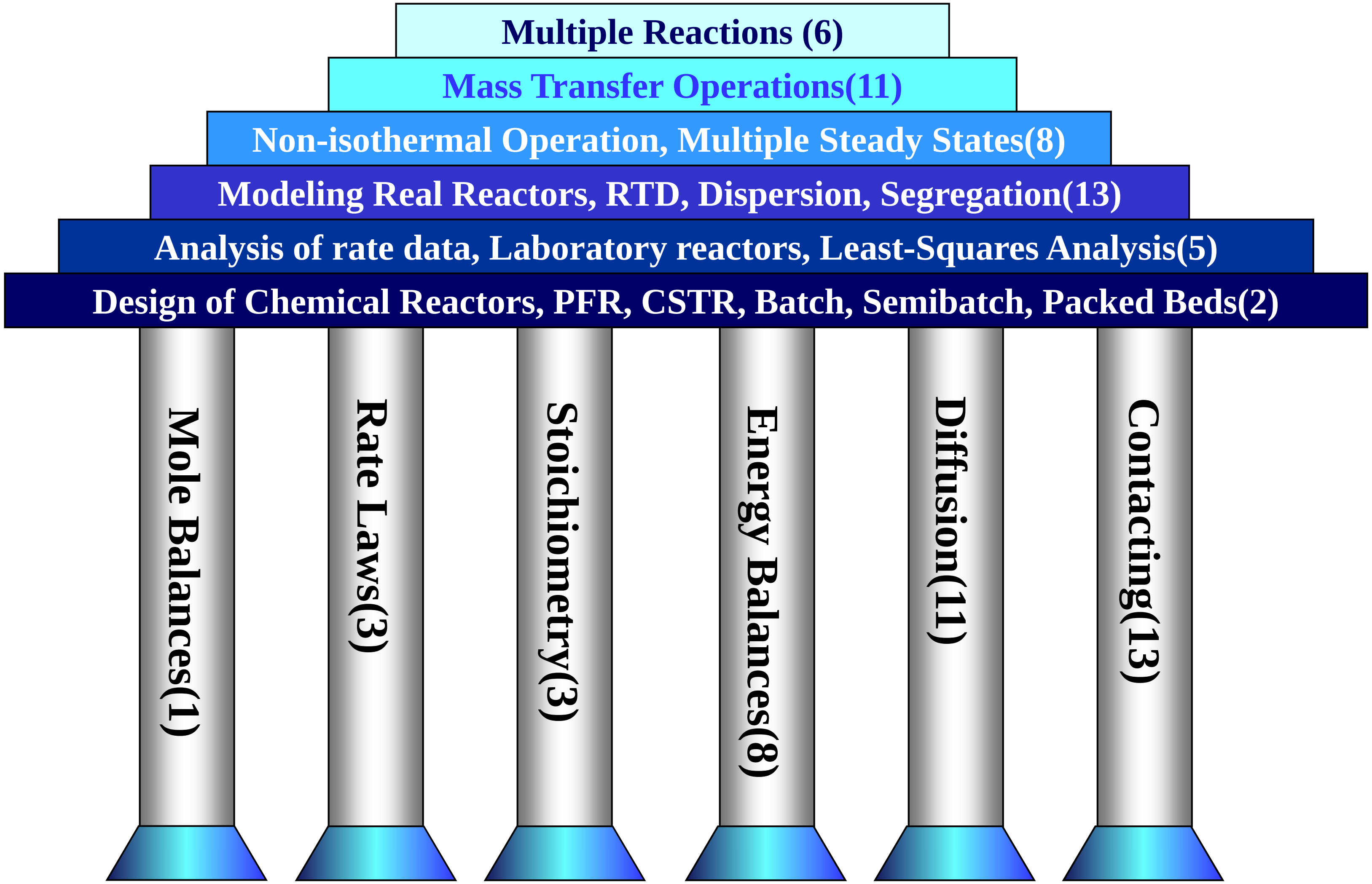
March 23, 19:00~21:00: **Quiz#1** (closed book)

April 25, 19:00~22:00: **Midterm Exam** (open text only)

May 16, 19:00~21:00: **Quiz#2** (closed book)

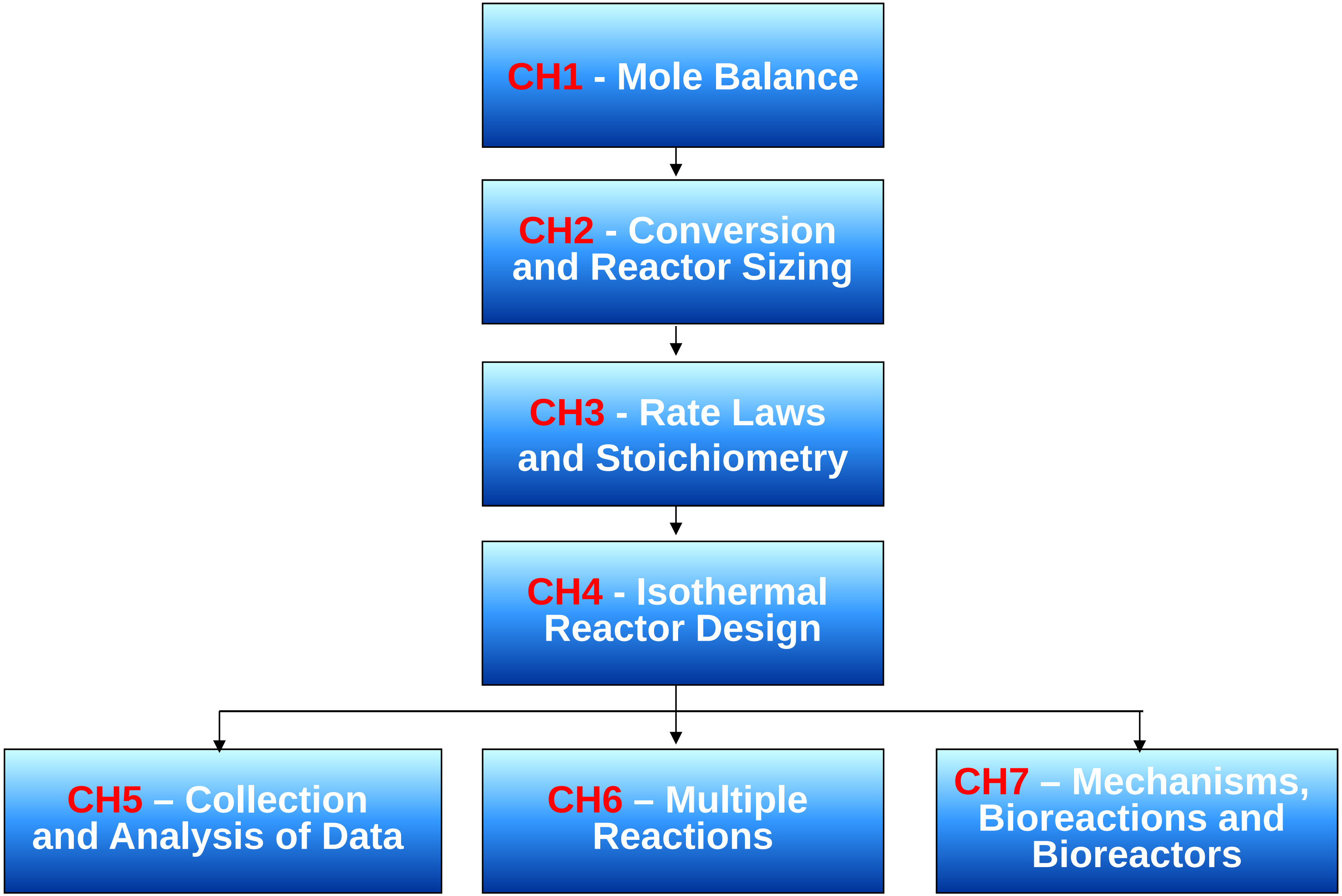
June 13, 19:00~22:00: **Final Exam** (open text only)

The Structure



Pillars of Chemical Reaction Engineering

Sequences for studying the text



How is a chemical engineer different from other engineers?

The knowledge of chemical reaction engineering

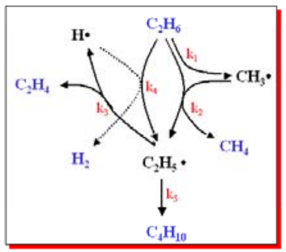
Chemical Kinetics

the study of
- chemical reaction rates
- reaction mechanisms

$$-r_A = kC_A$$

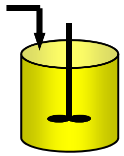
$$-r_A = kC_A^2$$

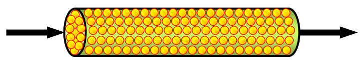
$$-r_A = \frac{k_1 C_A}{1 + k_2 C_A}$$



Reactor Design

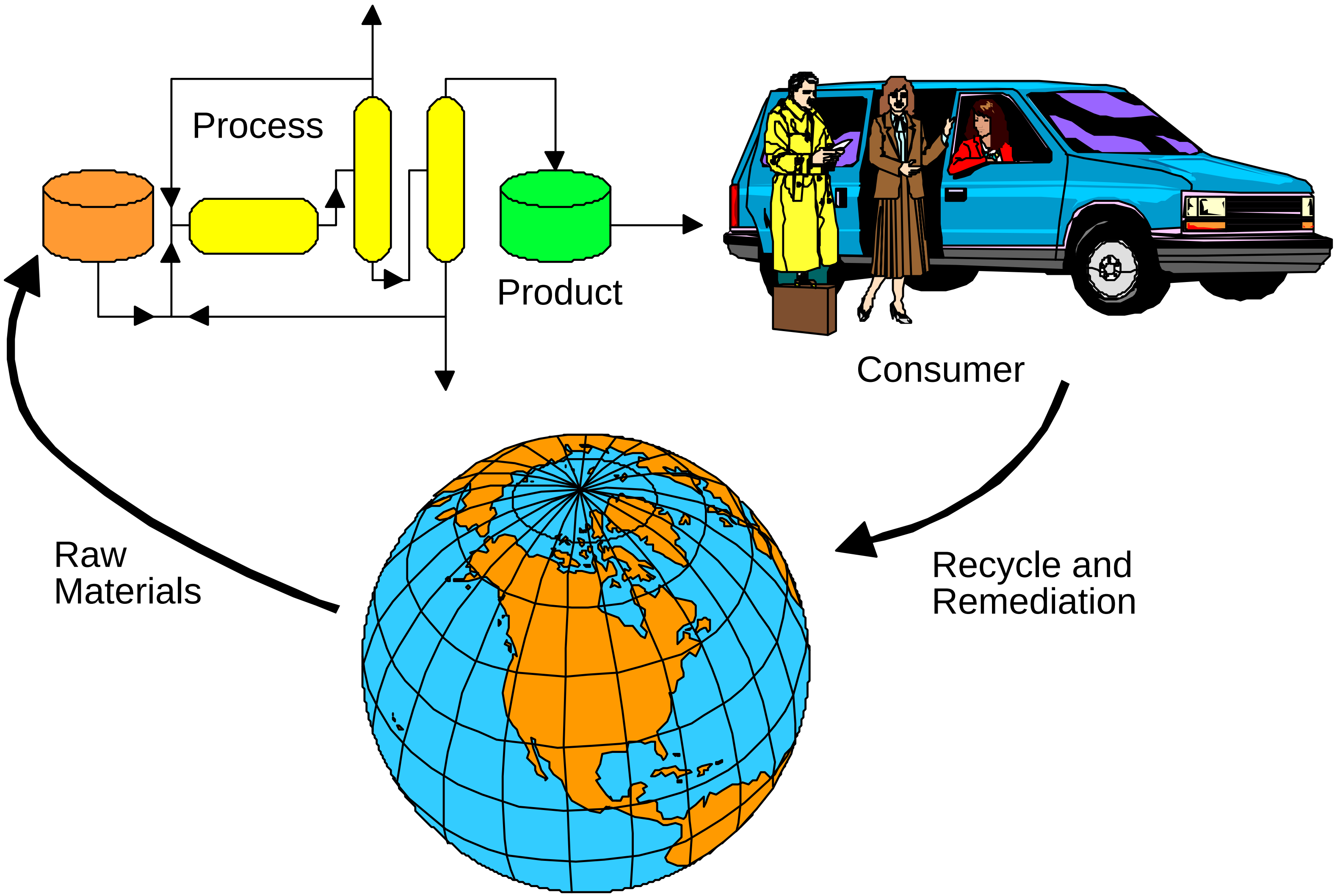
the study of
- Mole Balance
- Stoichiometry
- Fluid flow
- Heat & Mass Transfer
- Catalyst





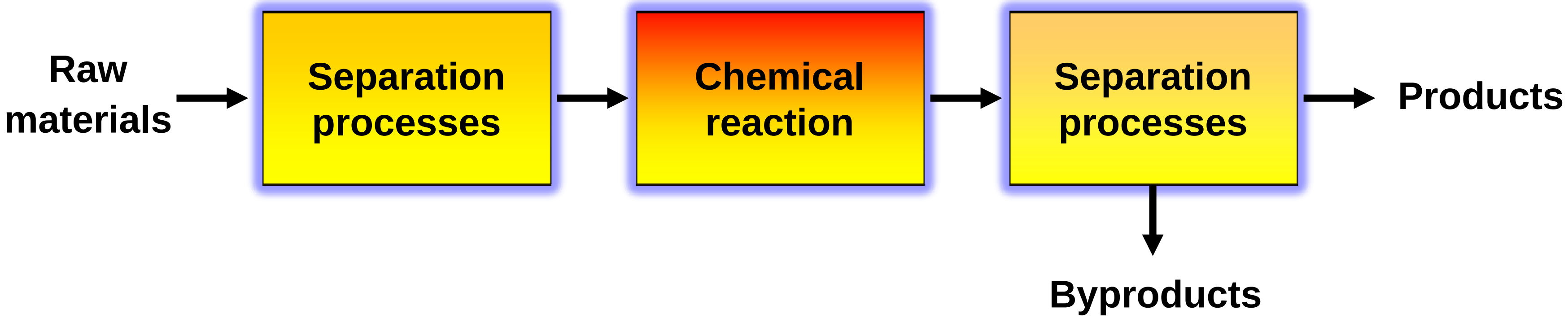
$$t = \int_{N_{A0}}^{N_A} \frac{dN_A}{r_A V}$$

Chemical Engineering - Working with the World



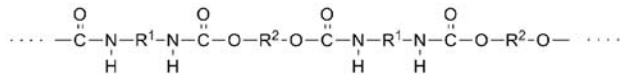
Chemical Process

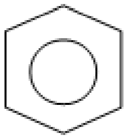
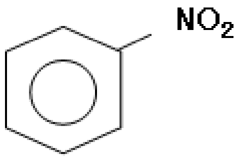
The key component is the chemical reactor in any processes.

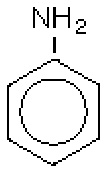


In typical chemical processes the capital and operating costs of the reactor may be only 10 to 25% of the total, with separation units dominating the size and cost of the process. Yet the performance of the chemical reactor totally controls the costs and modes of operation of these expensive separation units, and thus the chemical reactor largely controls the overall economics of most processes. Improvement in the reactor usually have enormous impact on upstream and downstream separation processes.

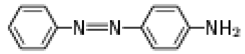
Use of Nitrobenzene





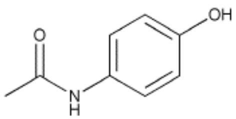
Benzene ➔ nitrobenzene ➔ aniline ➔ MDA ➔ MDI ➔ polyurethane



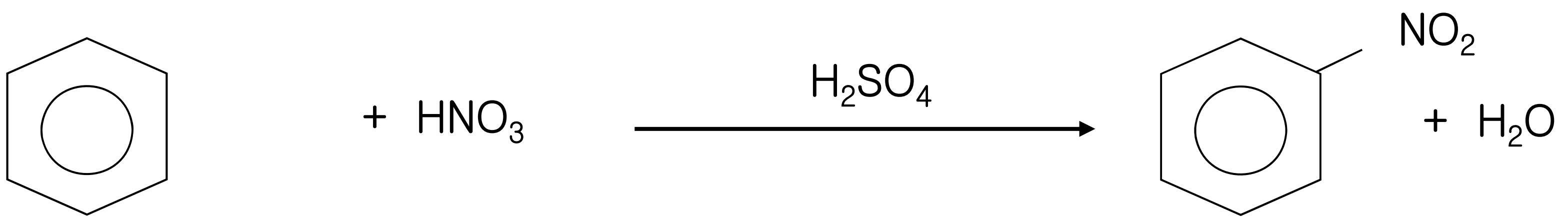
➔ **Herbicide, dye pigment**


➔ **Vulcanization accelerator**

Acetaminophen

The production of nitrobenzene: 1 ton/yr



Benzene	Nitric acid	Sulfuric acid	Nitrobenzene
M.W.=78	M.W.=63	M.W.=98	M.W.=123
bp=80°C	bp=121°C	bp=290°C	bp=211°C
SP.GR.=0.88	SP.GR.=1.4 (100%)	SP.GR.=1.5 (60%)	SP.GR.=1.2
Insoluble with water	soluble with water	soluble with water	Insoluble with water

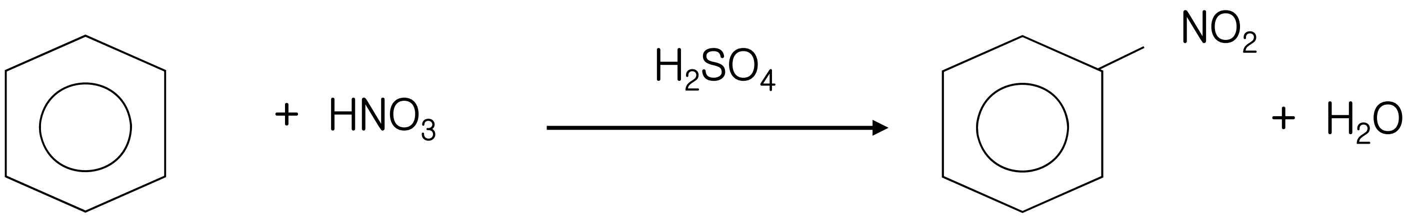
BASIS: 1000kg of Nitrobenzene

	Benzene	nitric acid	sulfuric acid	
Thoe.	8.13 kgmole	8.13 kgmole		8.13 kgmole
Theo.	634 kg	512 kg		1000 kg
Real	640 kg	515 kg	3.3 kg (consumption)	
Excess		3 kg	3.3 kg (consumption)	
Excess		0.037 kgmole	0.034 kgmole (consumption)	

$HNO_3 + NaOH \rightarrow NaNO_3 + H_2O$
$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

NaOH requirement=0.037*40+0.034*2*40=4.2kg ~ 0.004 ton

The production of nitrobenzene



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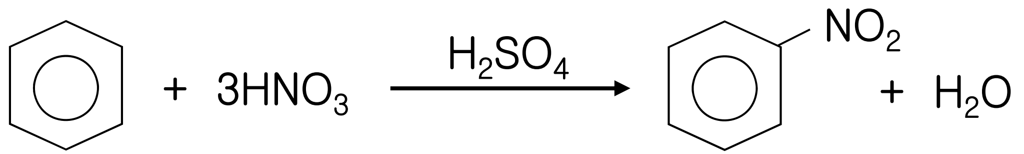
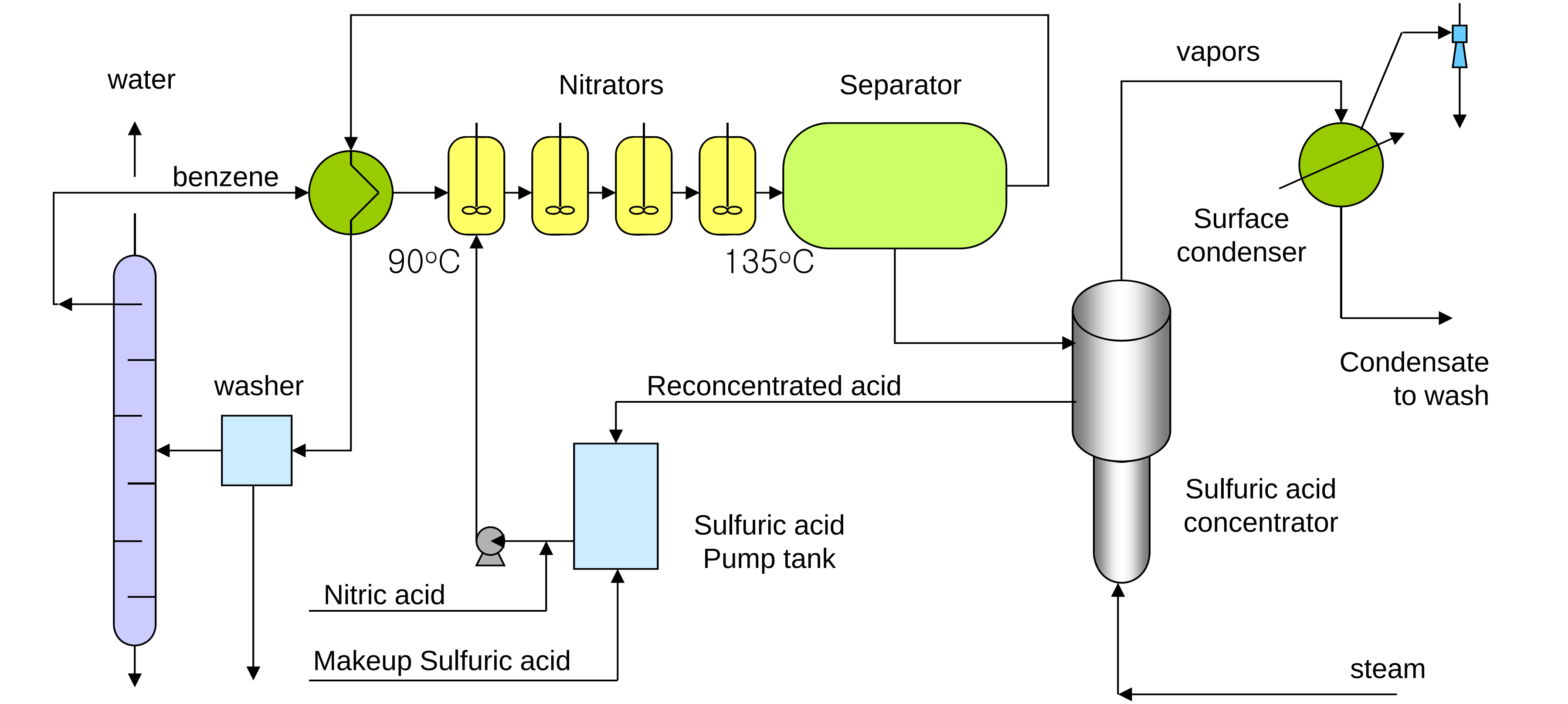
Insoluble with water	soluble with water	soluble with water	Insoluble with water

Nitrobenzene 1 ton

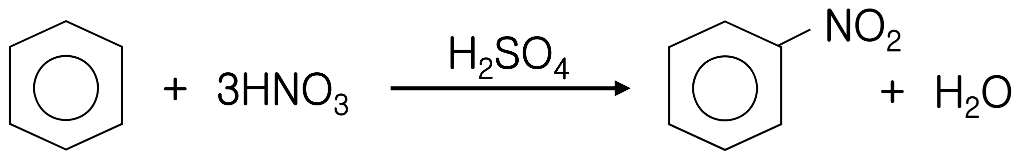
Raw materials			Utilities	
Benzene	0.64	ton	cooling water	14,200 gal
Nitric acid (100%)	0.515	ton	steam	800 lb
Sulfuric acid (100%)	0.0033	ton	electricity	20 kWh
NaOH	0.004	ton	compressed air	180 scf/m

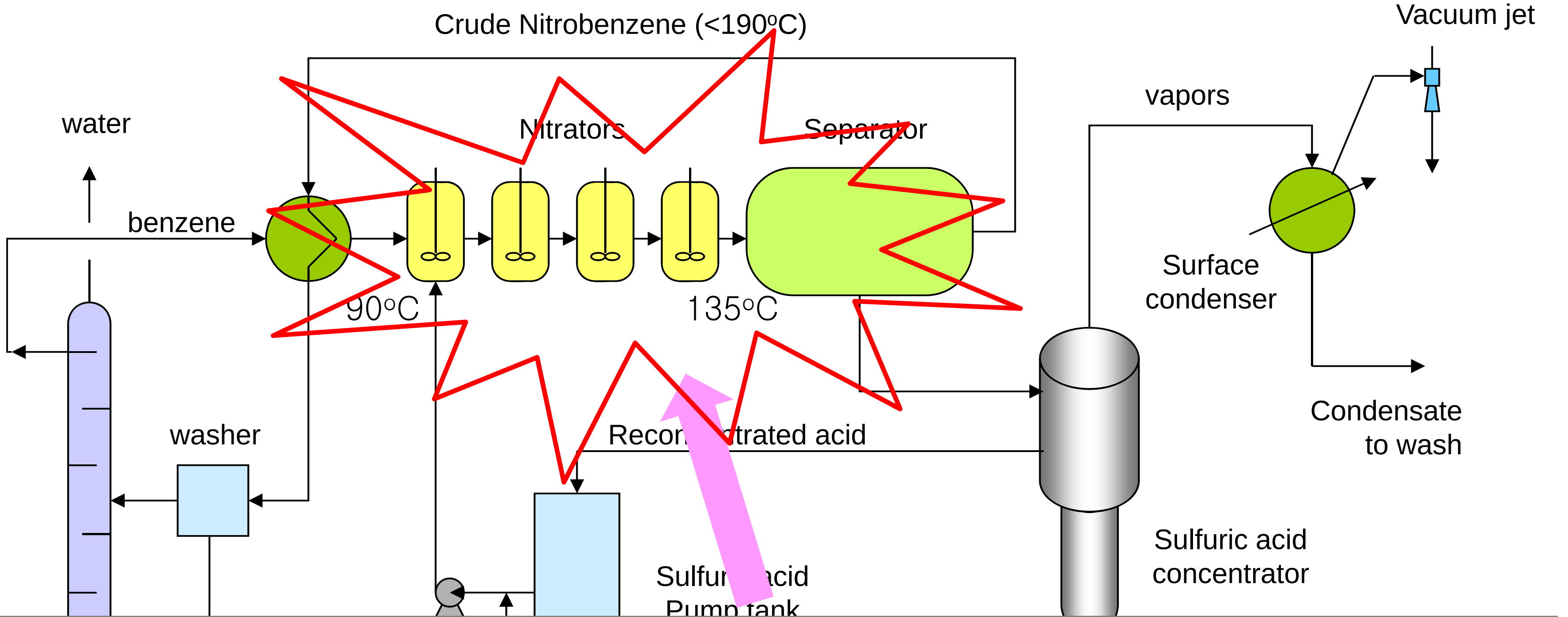
Flow sheet for the production of nitrobenzene





Flow sheet for the production of nitrobenzene





The goal of this course is to enable the student to develop a clear understanding of the fundamentals of chemical reaction engineering. The students are able to derive and solve steady-state and transient material balance with reactions. To learn how to apply the fundamental principles of chemical kinetics to the design of chemical reactors for both homogeneous and heterogeneous cases. To provide an integrated study of fundamentals and quantitative design techniques of batch and flow chemical reactors applying fundamental knowledge of mathematics, science and engineering.