# UNIVERSITY OF LAGOS

## Chemical Engineering Department

## 2021/2022 SESSION, 2nd SEMESTER

# CHG 502: Optimization of Chemical Processes

## Practice Problems, Set - I (PPS_I)

### Problem Formulation
### &
### Least Square Optimization

**Date Given:** Monday, February 27, 2023
**Date Due:** Friday, March 17, 2023
**Proposed Test date:** March 22nd, 9:00 -10:00am

# Why teamwork?

**The essence of forming teams is to foster intra- and inter- teamwork, working together as a team while at the same time relating with other teams.**

*The team supports its members and its members support the team – all for one, and one for all*

**"Great things in business are never done by one person. They're done by a team of people."**

- Steve Jobs

**"Individual commitment to a group effort – that's what makes a team work, a company work, a society work, a civilization work."**

- Vince Lombardi

**"The strength of the team is each individual member. The strength of each member is the team."**

- Phil Jackson

**"Teamwork divides the task and multiplies the success."**


[Please find the teams for PPS-1 on the last page]

# *Modus Operandi*

1. Someone in the group should spearhead the coming together of the group, either via whatsapp, zoom, or any of the social media platforms.
2. At the first meeting of the group, choose a group leader and an assistant, they will coordinate the affairs of the group.
3. Submit the practice problem on or before the deadline, with the front page showing team members and their signature. The team leader and the assistant are to score each student's participation, over 10, before finally submitting to me.
4. On the last page of the submission, is a grid where each team member honestly scores the other team members for participation, over 10, there shall be no self scoring – see example below for Group 1

| **Group Members** | 170401513 Adebayo Samuel | 160401039 Adeniyi Adeyosola | 160401067 Akaforonye Johnpaul | 170401520 Chijioke Favour | 160401033 Ibrahim Ibrahim Christopher | 150401018 Musa Mohammed | 160401008 Obafemi Oluwadolapo | 160401058 Okafor Onyeka Peter | 170401501 Oladeji Ooreoluwa | 160401017 Onigemo Oluwatimilehin |
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| 170401513 Adebayo Samuel | | | | | | | | | | |
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| 160401008 Obafemi Oluwadolapo | | | | | | | | | | |
| 160401058 Okafor Onyeka Peter | | | | | | | | | | |
| 170401501 Oladeji Ooreoluwa | | | | | | | | | | |
| 160401017 Onigemo Oluwatimilehin | | | | | | | | | | |

# On Problem Formulation

**Question 1.1 – 1.6 (Edgar,Himmelblau and Lasdon)**

**Question 1.2 – 1.8 (Edgar,Himmelblau and Lasdon**

**Question 1.3 – 1.13 (Edgar,Himmelblau and Lasdon**

**Question 1.4**

In a chemical plant, the cost of pipes, their fittings, and pumping are important investment cost. Consider the design of pipeline L metres long that should carry fluid at the rate of Q $m^3$/s. The selection of economic pipe diameter D (cm.) is based on minimizing the annual cost of pipe, pump, and pumping. Suppose the annual cost of a pipeline with a standard carbon steel pipe and a motor-driven centrifugal pump can be expressed as:

$$f = 0.45L + 0.245LD^{1.5} + 3.25(hp)^{1/2} + 61.6(hp)^{0.925} + 102$$

where

$$hp = 4.4\times10^{-8}\frac{LQ^3}{D^5} + 1.92\times10^{-9}\frac{LQ2.68}{D^{4.68}}$$

Formulate the optimization problem for designing a pipe of length 1000 m with a fluid rate of 20 $m^3$/s. The diameter of the pipe should be in the range of 0.25 to 6 cm

**Question 1.5**

We are interested to produce P in the reaction $A \rightarrow P$ using a continuous reactor at $v$ = 240 litres/ hr with $C_{Ao}$ = 3 moles/liter. However, it is noticed that there is a second reaction $P \rightarrow R$ that can also occur. This undesired reaction produced undesired product $R$. It is found that both reactions are irreversible and first order with $k_1$. = 0.45 $min^{-1}$ and $k_2$. = 0.1 $min^{-1}$. Formulate the optimization problem for finding maximum yield of $P$.

**Question 1.6**

A chemical plant has received an order for 400 liters of alcohol with the constraints that the alcohol must contain 4 percent methanol by volume, and it must be supplied immediately. The company wishes to fill the order, but does not have 4 percent methanol in stock. It is decided to mix two different compositions of methanol now in stock to give the desired final product. One of the alcohol in stock(alcohol A) contains 4.5 percent methanol by volume and is valued at $0.09 per liter. The other alcohol in stock (alcohol B) contains 3.7 percent methanol by volume and is valued at $0.07 per liter. Water (W) can be added to the blend at no cost. What volume combination of the two alcohols in stock with water, including at least 40 liters of alcohol A, will give the minimum ingredient cost for the 400 liters of 4 percent methanol?

**Question 1.7**

Topological optimization, which is about the physical layout of the plant, has the greatest effect on the overall profitability of the plant, and is therefore done before parametric optimization (which is the manipulation of decision variables).

The layout of a chemical process plant is shown in Fig. 1. This plant consists of a water tank ($T$). a pump ($P$), a fan ($F$), and a compressor ($C$). The positions of the different units are also indicated in the figure in terms of their ($x$, $y$) coordinates. It has been decided to add a new heat exchanger ($H$) within this plant. Addition of new unit may cause congestion within the plant. It is decided to place $H$ within a rectangular area given by $\{-15 \le x \le 15, -10 \le y \le 10, \}$ to avoid congestion. Formulate the optimization problem to find the position of $H$ to minimize the sum of its distances $x$ and $y$ from the existing; units, T, $P$, $F$, and $C$.

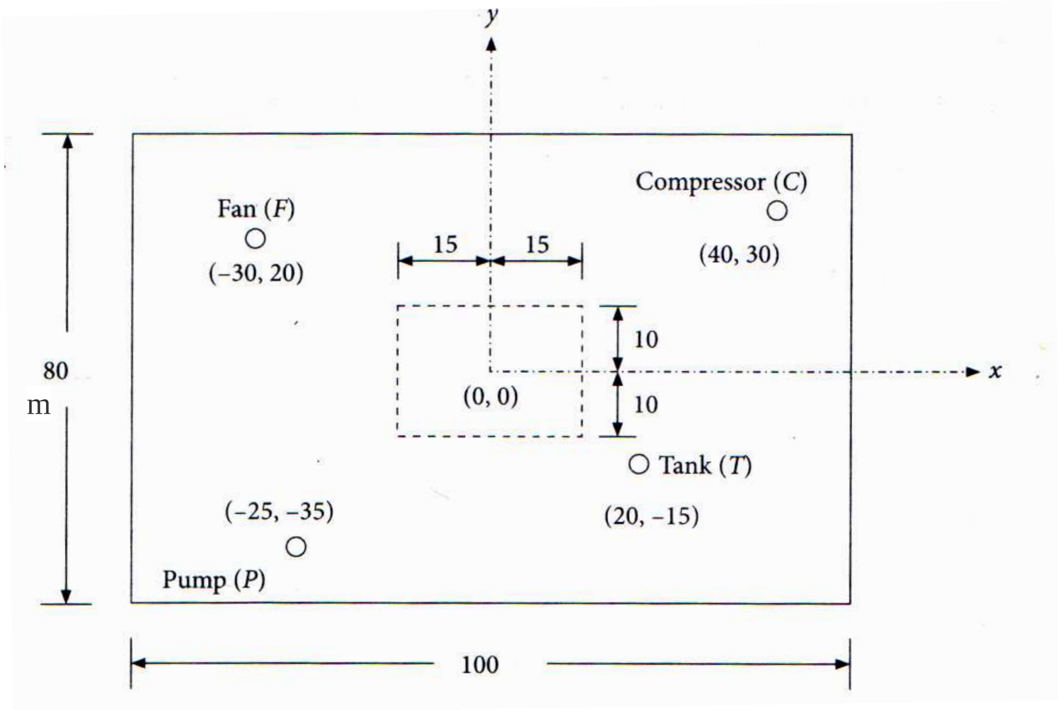



**Figure 1** Layout of a chemical processing plant (coordinates in m)

**Question 1.8**

A certain plant can manufacture 5 different products in any combination. Each product requires time on each of three machines in the following manner (all numbers are in minutes/unit):

| Product | Machine 1 | Machine 2 | Machine 3 |
|---|---|---|---|
| *A* | 12 | 8 | 5 |
| *B* | 7 | 9 | 10 |
| *C* | 8 | 4 | 7 |
| *D* | 10 | 0 | 3 |
| *E* | 7 | 11 | 2 |

Each machine is available 128 hours per week. Products $A$, $B$, and $C$ are purely competitive, and any amounts made may be sold at respective prices of \$5, \$4, and \$5. The first 20 units of $D$ and $E$ produced per week can be sold at \$4 each, but all made in excess of 20 can only be sold at \$3 each. Variable labor costs are \$4 per hour for machines 1 and 2 and \$3 per hour for machine 3. Material costs are \$2 for products $A$ and $C$, and \$1 for products $B$, $D$, and $E$. You wish to maximize profit to the firm. Formulate the optimization problem and classify it.

**Question 1.9**
It is desired to cool a gas [$C_p$ = 0.3 Btu/lbm-$^o$F] from 195 to 90 $^o$F, using cooling water [$C_p$ = 1.0 Btu/lbm-$^o$F, ρ= 62.4 lbm/ft$^3$] at 80 $^o$F in a counter-current heat exchanger. Water costs $0.20/1000 ft3, and the annual fixed charges for the exchanger are $0.50/ft$^2$ of heat transfer area. The heat transfer coefficient is $U$ = 8 Btu/hr-ft$^2$-$^o$F for a gas rate of 3000 lbm/hr. The heat exchanger is operated 365 days/year (24 hours/day).
Formulate this heat exchange operation as an optimization problem to minimize the total annual cost and classify it.

**Hint:** $\Delta T_{lm} = \log\text{-mean } \Delta T = (\Delta T_2 - \Delta T_1)/\text{In } (\Delta T_2/\Delta T_1)$

where $\Delta T_2$ and $\Delta T_1$ are the terminal temperature differences of heat exchanger.

**Question 1.10**
An organic chemical is being produced by a batch operation in which no product is obtained until the batch is finished. Each cycle consists of the operating time necessary to complete the reaction plus an additional time of 1.4 h required for discharging and charging. The operating time per cycle is equal to $1.5P_b^{0.25}$, where $P_b$ is the kilogram of product produced per batch. The operating costs during the operating period are $20 per hour, while the costs during the discharge-charge period are $15 per hour. The annual fixed costs $C_F$ for the equipment vary with the size of the batch in the following manner: $C_F = 340P_b^{0.8}$ $/yr.
Inventory and storage charges may be neglected. If necessary, the plant can be operated 24 h/day for 300 days/yr. The annual production is 10$^6$ kg of product. At this capacity, raw material and miscellaneous costs, other than those already mentioned, amount to $260,000 per year. Formulate the optimization problem to determine the cycle time for conditions of minimum total cost per year.

**Question 1.11**
As a chemical engineer, you've been asked to design and determine the radius *r* and the height *h* of a right-circular cylinder of largest volume that can be inscribed in a right-circular cone with a radius of 6 meters and a height of 10 meters as shown figure 2 below. Also compute this maximum volume of the cylinder and prove that volume calculated is a maximum.

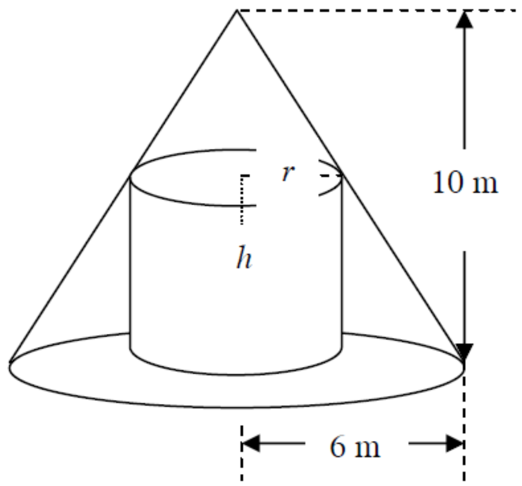



**Figure 2**

**Question 1.12**

A refinery has four different crudes which are to be processed to yield four products: gasoline, heating oil, jet fuel, and lube oil. There are maximum limits both on product demand (what can be sold) and crude availability. A schematic of the processing operation is shown in Figure 3 below::

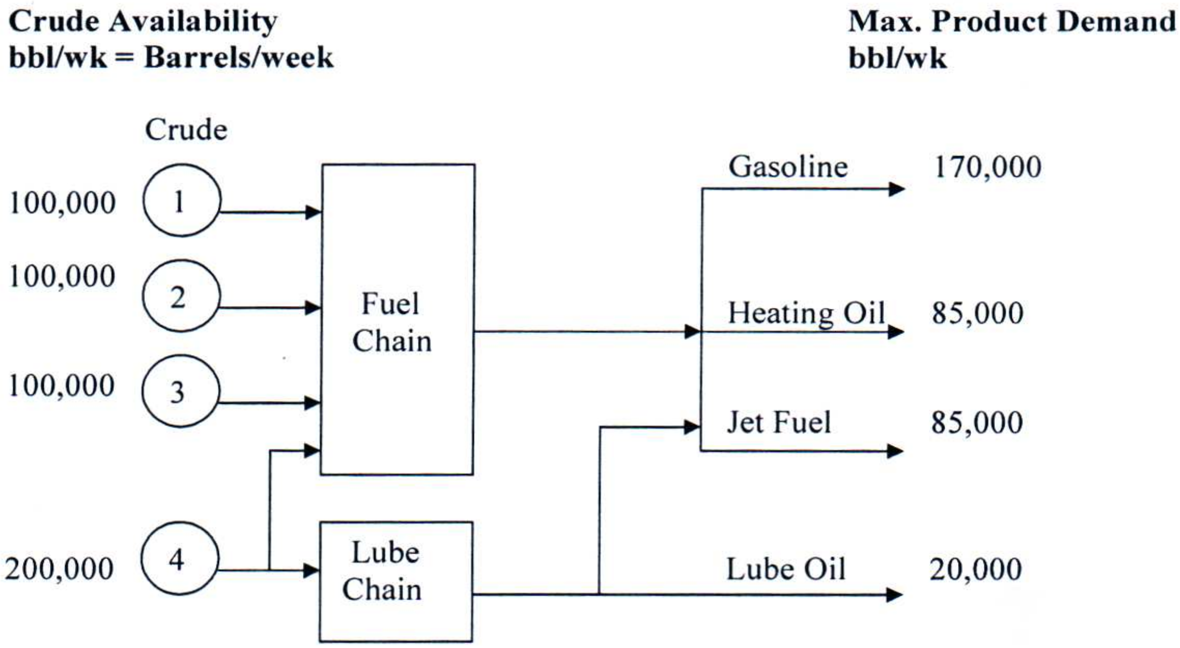



**Figure 3.** Schematic of raw materials/products for Question B1

Given the tabulated profits, costs and yields in Table 1 below,

a) **Formulate the problem** as an optimization problem that maximizes profit. [Hint: $x_i$, where $i = 1,2,3$ are bbl/wk of crude type $i$ through process fuel chain, $x_4$ and $x_5$ are bbl/wk of crude type 4 through process fuel and lube chains respectively]

b) What method will you use to solve this type of optimization problem and why?

**Table 1 Profits, Costs and Yield Data for Figure 3**

| | | Crude Type | | | | | Product Value $/bbl |
|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 | | |
| | | | | | Fuel Process | Lube Process | |
| **Yields** bbl product per bbl crude) | Gasoline | 0.6 | 0.5 | 0.3 | 0.4 | 0.4 | 45.00 |
| | Heating oil | 0.2 | 0.2 | 0.3 | 0.3 | 0.1 | 30.00 |
| | Jet fuel | 0.1 | 0.2 | 0.3 | 0.2 | 0.2 | 15.00 |
| | Lube Oil | 0 | 0 | 0 | 0 | 0.2 | 60.00 |
| | Others* | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | |
| | Crude cost** | 15.00 | 15.00 | 15.00 | 25.00 | 25.00 | |
| | Operating cost ** | 5.00 | 8.50 | 7.50 | 3.00 | 2.50 | |

*Losses in processing, ** Costs are in $/bbl

**Question 1.13**
To reduce heat losses, the exterior flat wall of a furnace is to be insulated. To determine the optimum insulation thickness, it is necessary to consider and balance the costs of the insulation and the value of the energy saved by adding the insulation. The rate of heat transfer *Q* through the wall is:

$$Q = UA(T_{furnace} - T_{wall})$$

where *T* is in $^oF$ and *Q* is in Btu/hr. The overall heat transfer coefficient *U* is related to the outside convective heat transfer coefficient *h* and the thermal conductivity of insulation *k* by:

$$\frac{1}{U} = \frac{1}{h} + \frac{t}{12k}$$

where *t* is the thickness in inches of the insulation.

It is desired to maximize the savings in total operating cost, savings expressed as the difference between the dollar value of the heat conserved minus the cost of the insulation over a span of 5 years (after that, the insulation will have to be replaced).
Formulate this problem as an optimization problem, classify it, and obtain the optimum value of *t* (in inches) using the following data:

| | |
|---|---|
| Temperature inside the furnace | 500 $^oF$ (constant) |
| Air temperature outside wall | Assume constant at 70$^oF$ |
| Heat transfer coefficients: | |
| Outside air film *h* | 4.0 Btu/(hr)(ft$^2$)($^oF$) |
| Conductivity of insulation *k* | 0.03 Btu/(hr)(ft)($^oF$) |
| Total cost of insulation | \$0.75/(ft$^2$)(per inch of thickness) |
| (per unit area per inch of thickness) | |
| Values of energy saved | \$0.60/10$^6$ Btu |
| (i.e. the dollar difference between adding insulation and having no insulation for every 1 million Btu is \$0.60.) | |
| Hours of operation | 8700 hours/year |

Prove that your optimum *t* is a maximum. **Hint:** The heat transfer area *A* is constant.

**Question 1.14**
Distillation is a widely used separation technique in the chemical process industries: it is an energy intensive process, therefore optimization of a distillation process is about minimi**zing energy, for a given degree of separation. Factors that affect energy are the number** of stages, N, the reflux ratio, R and the feed location. The total cost is made up of the annual operating cost (heating medium to produce vapour and cooling medium for condensation) and the annual fixed charges ( this takes into account interest, depreciation on installed cost of column, condenser, reboiler and maintenance)

For the distillation column shown in Fig. 4

$$V = L + D$$

$$= RD + D = (R+1)D = \left(\frac{R_m R}{R_m} + 1\right) D \qquad [1]$$

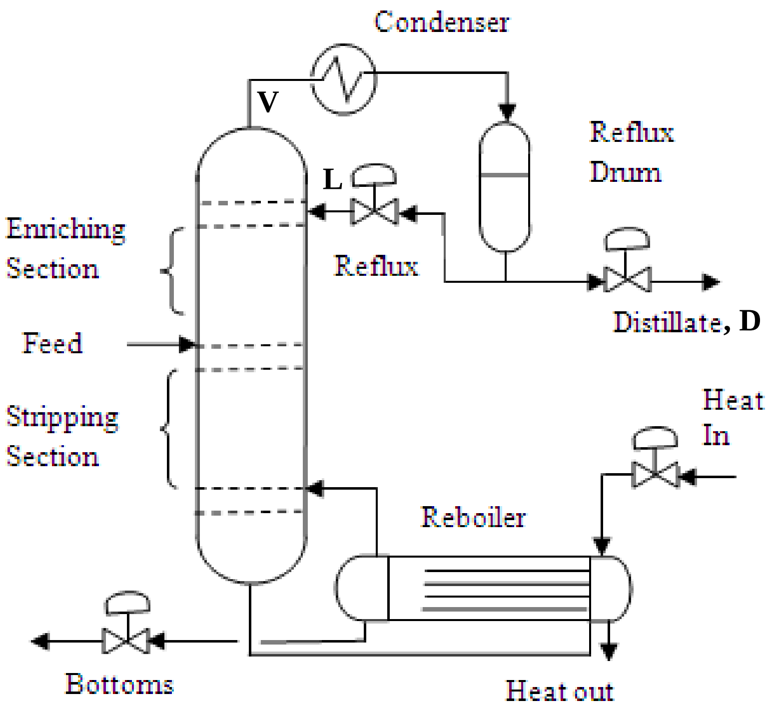



**Figure 4.** A typical; distillation column

For a binary mixture, assuming saturated liquid feed

$$R_m \sim \frac{1}{(\alpha-1)x_F}$$

and assuming complete recovery of light components, $D \approx Fx_F$ , and equation [1] above can be rewritten as:

$$V = \left[\frac{R/R_m}{(\alpha-1)x_F} + 1\right]Fx_F$$

the vapour rate, in the rectifying section, is now written in terms of known quantities. Given the design equations, process information and cost indices below, plot the individual cost models, and the total cost as a function of $R/R_m$ . What reflux ratio minimizes the total cost?

**Design equations are**:

$$N = \frac{N_T}{E_o}$$

$$H_T = \frac{2N}{E_o} + H_o$$

$$D_T = 0.0164\sqrt{V\left[379M_G\left(\frac{T_b}{520}\right)\left(\frac{14.7}{P_T}\right)\right]^{1/4}}$$

**Process information**:

$$\text{Feed rate} = 200 \text{ mol/hr}, \; x_F = 0.50, \; x_D = 0.99,$$

$$\alpha = 2.0, \; E_o = 0.5, \; H_o = 15\text{ft}, \; \Delta H_v = 13{,}300 \text{ Btu/mol}$$

$$U_c = 100 \text{ Btu/(hr.ft}^2.^{\circ}\text{F)}, \; \text{T}_b = 177\,^{\circ}\text{F}, \; \text{P}_T = 15 \text{ psia}$$

$$M_G = 92, \; \text{M\&S} = 850$$

**Nomenclature** $x_F$, feed composition of light key, $x_D$, distillate composition, α, relative volatility, $E_o$,, overall plate efficiency, $H_o$, space at the ends of the column for vapour disengagement and the liquid sump, $\Delta H_v$, heat of vapourization of light key, $U_c$, condenser overall heat-transfer coefficient, $T_b$ , bubble point, $P_T$, total pressure, $M_G$, molecular weight of gas, M&S, Marshall &Swift cost index compensation factor, $N_T$, theoretical number of columns, $N$, actual number of columns, $H_T$, height of distillation column.

The **cost models for a distillation column** are given by:

Column cost:= $$\frac{\text{M\&S}}{280}(3.28)(101.9)D_T^{1.06}\,H_T^{0.802}\big/3$$

Condenser = $$\frac{\text{M\&S}}{280}(3.29)(101.3)\left(\frac{\nabla H_v}{U\Delta T_m}\right)^{0.65} V^{0.65}\big/3$$

Assume cooling water is available at 90°F and returned at 120°F

Reboiler = $$\frac{\text{M\&S}}{280}(3.29)(101.3)\left(\frac{\nabla H_v}{11{,}250}\right)^{0.65} V^{0.65}\big/3$$

Steam = $$\left(\frac{3}{1000}\right)\left(\frac{\nabla H_v}{933}\right)(8150)V$$

Cooling water = $$\left(\frac{0.06}{1000}\right)\left(\frac{1}{8.34}\right)\left(\frac{\nabla H_v}{30}\right)(8150)V$$

**Question 1.15**

A condenser for a distillation unit must be designed to condense 2300 kg of vapor per hour. The effective condensation temperature for the vapor is 77°C. The heat of condensation for the vapor is 465 kJ/kg. The cost of the cooling water at 21°C is \$2.56 per 100 m$^3$. The overall heat-transfer coefficient at the optimum conditions may be taken as 0.284 kJ/(m$^2$.s.K). The cost for the installed heat exchanger is \$380 per square meter of heat-transfer area, and annual fixed charges including maintenance are 20 percent of the initial investment. The heat capacity of the water may be assumed to be constant at 4.2 kJ/(kg.K). If the condenser is to operate 6000 h/yr,. Formulate the optimization problem to determine the cooling water flow rate, in kilograms per hour, for optimum economic conditions.

Notes:

If a condenser, with water as the cooling medium, is designed to carry out a given duty, the cooling water may be circulated at a high rate with a small change in water temperature or at a low rate with a large change in water temperature. The temperature of the water affects the temperature-difference driving force for heat transfer. Use of an increased amount of water, therefore, will cause a reduction in the necessary amount of heat-transfer area and a resultant decrease in the original investment and fixed charges. On the other hand, the cost for the water will increase if more water is used.
An economic balance between conditions of high water rate and low surface area, and low water rate and high surface area, indicates that the optimum flow rate of cooling water occurs at the point of minimum total cost for cooling water and equipment fixed charges.

Consider the general case in which heat must be removed from a condensing vapor at a given rate designated by q in kJ/s. The vapor condenses at a constant temperature of $T_{cond}$, and cooling water is supplied at a temperature $T_1$. The rate of heat transfer can be expressed as

$$\dot{q} = \dot{m}C_p(T_2 - T_1) = UA\Delta T_{\text{log mean}} = \frac{UA(T_2 - T_1)}{\ln[(T_{cond} - T_1)/(T_{cond} - T_2)]}$$

where $\dot{m}$ is the flow rate of cooling water, $C_p$ the heat capacity of the cooling water, $T_2$ the temperature of the cooling water leaving the condenser, $U$ the constant overall heat-transfer coefficient determined at optimum conditions, and $A$ the area of heat transfer. Solving the equation above for the flow rate of cooling water gives

$$\dot{m} = \frac{\dot{q}}{C_p(T_2 - T_1)}$$

The design conditions set the values of $\dot{q}$ and $T_1$ and the heat capacity of water generally can be approximated as 4.2 kJ/(kg-K). The equation above shows that the flow rate of the cooling water is fixed if the temperature of the water leaving the condenser is fixed. Under these conditions, the optimum flow rate of cooling water can be found directly from the optimum value of $T_2$.
The annual cost for cooling water is $\dot{m} H_y C_w$, where $H_y$ designates the number of hours of condenser operation per year and $C_w$ the cooling water cost, assumed to be directly proportional to the amount of water supplied.' The annual fixed charges for the condenser are $AK_F C_A$, where $K_F$ is the annual fixed charge including maintenance expressed as a fraction of the initial cost for the installed equipment and $C_A$ the installed cost of the condenser per square meter of heat-transfer area.

## Question 1.16

A sieve-plate distillation column is being designed to handle 318 kg mol of feed per hour. The unit is to operate continuously at a total pressure of 1 atm. The feed contains 45 mol percent benzene and 55 mol percent toluene, and the feed enters at its boiling temperature. The overhead product from the distillation tower must contain 92 mol percent benzene, and the bottoms must contain 95 mol percent toluene. Determine the following:

(a) The optimum reflux ratio as mols of liquid returned to tower per mol of distillate product withdrawn.
(b) The ratio of the optimum reflux ratio to the minimum reflux ratio.
(c) The percent of the total variable cost due to steam consumption at the optimum conditions.

The following data apply:

- Vapor-liquid equilibrium data for benzene-toluene mixtures at atmospheric pressure are presented below (see plot on next page)
- The molal heat capacity for liquid mixtures of benzene and toluene in all proportions may be assumed to be 1.67 x 105 J/(kg mol.K).
- The molal heat of vaporization of benzene and toluene may be taken as 3.2 x $10^4$ kJ/kg mol.
- Effects of change in temperature on heat capacity and heats of vaporization are assumed negligible.
- Heat losses from the column are negligible. Effects of pressure drop over the column may be neglected.
- The overall coefficient of heat transfer is 0.454 kJ/($m^2$.s.K) in the reboiler and 0.568 kJ/($m^2$.s.K) in the condenser.

- The boiling temperature is $94^0$C for the feed, $81.7^0$C for the distillate, and $108^o$C for the bottoms. The temperature-difference driving force in the reflux condenser may be based on an average cooling water temperature of $32.2^0$C, and the change in cooling water temperature is $27.8^0$C for all cases. Saturated steam at 415 kPa is used in the reboiler. At this pressure, the temperature of the condensing steam is $144.8^0$C, and the heat of condensation is $2.13 \times 10^3$ kJ/kg. No heat-saving devices are used.
- The column diameter is to be based on a maximum allowable vapor velocity of 0.76 m/s at the top of the column. The overall plate efficiency may be assumed to be 70 percent. The unit is to operate 8500 h/yr.

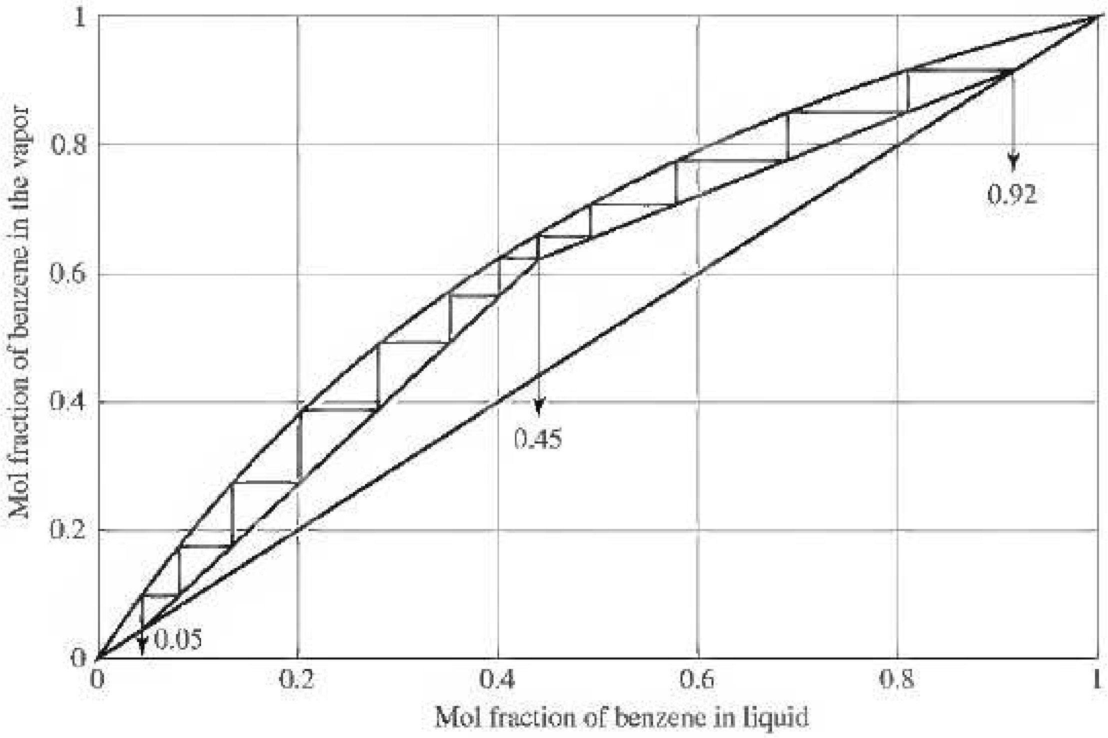



**Figure 5**. Vapor-liquid equilibrium data for benzene-toluene mixtures at atmospheric pressure

- **Cost Data**

Steam = \$3.31 per $10^3$ kg
Cooling water = \$0.0238 per $10^3$ kg

The sum of costs for piping, insulation, and instrumentation can be estimated to be 60 percent of the cost for the installed equipment. Annual fixed charges amount to 15 percent of the total cost for installed equipment, piping, instrumentation, and insulation.
The following costs for the sieve-plate distillation column, condenser, and reboiler are for installed equipment and include delivery and erection costs. To simplify the calculations, all equipment costs may be interpolated.

| Sieve-plate distillation column | | Condenser, tube-and-shell heat exchanger | | Reboiler, tube-and-shell heat exchanger | |
|---|---|---|---|---|---|
| Diameter, m | \$/plate | Heat-transfer area, $m^2$ | Cost, \$ | Heat-transfer area, $m^2$ | Cost, \$ |
| 1.50 | 2640 | 75 | 21,100 | 90 | 37,200 |
| 1.75 | 3170 | 95 | 24,600 | 130 | 45,700 |
| 2.0 | 3910 | 110 | 27,000 | 165 | 52,700 |
| 2.25 | 4730 | 130 | 29,800 | 200 | 59,100 |
| 2.5 | 5680 | 150 | 32,250 | 240 | 65,200 |

**Question 1.17**

Carbon dioxide under pressure is dissolved in carbonated drinks by gas absorption, so that when the pressure is subsequently released on opening the container, effervescence occurs. 'Biggie fizzy drinks' has an absorption column containing wooden grids, which is to be used for absorbing $CO_2$ into the company's BiGi-Cola. A mixture of air and $CO_2$ will enter the column at a rate of 2 $m^3$/min, temperature 25°C, and pressure of 1.1 atm. The concentration of $CO_2$ in the entering gas is specified and a given fraction of the entering $CO_2$ must be absorbed into the drink. The molecular weight of the entering gas mixture may be assumed to be 30 $gmol^{-1}$. Under the specified design conditions, the number of transfer units necessary varies with the superficial gas velocity (velocity in the empty column) as follows:

$$\text{Number of transfer units, NTU} = 0.32G_s^{0.18}$$

where $G_s$ is the entering gas velocity as kg/(hr-$m^2$) based on the cross-sectional area of the empty column. The height of a transfer unit, HTU, is constant at 5 m. The initial cost of the installed column is ₦500/$m^3$ of inside volume, and annual fixed charges, amount to 20% of the initial cost. Variable operating charges of the absorbent, blower power, and pumping power are represented by the following equation:

$$\text{Total variable operating cost, ₦/hr} = 1.8\times10^{-8}G_s^2 + \frac{81}{G_s} + \frac{4.8}{G_s^{0.8}}$$

The unit is to operate 6,000 hr/year.
The company desperately needs to operate at minimum total annual cost.

**Formulate this problem** as an optimization problem to minimize the total annual cost.

The following information might be useful

- *Height of column, H = HTU x NTU*
- *Column is a vertical cylinder with a diameter, D and a height, H.*
- *Total annual cost = Annual fixed charges + Annual variable operating charge*
- *Independent design (decision) variable is the superficial gas velocity,* $G_s$
- *For the ideal gas law, PV=nRT, gas constant,* $R = 8.205\,746 \times 10^{-5}\,m^3\,atm\,K^{-1}mol^{-1}$

**Question 1.18 – 1.24 (Edgar, Himmelblau and Lasdon)**

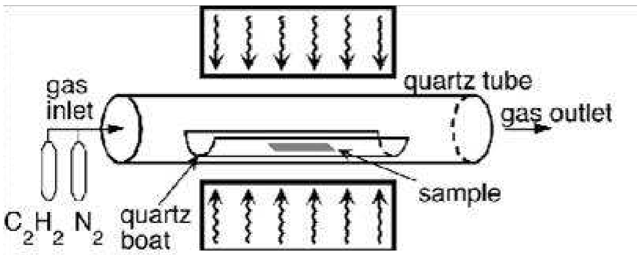
# On Least Square Optimization

**Question 1.19 – 2.9 (Edgar, Himmelblau and Lasdon)**

**Question 1.20 – 2.10 (Edgar, Himmelblau and Lasdon)**

**Question 1.21 – 2.20 (Edgar, Himmelblau and Lasdon)**

**Question 1.22**
Chemical Vapour Deposition (CVD) is a vacuum deposition method used to produce high quality, high performance solid materials, and often used in the semiconductor industry to produce thin films. Gaseous precursors react to form a solid coating on a heated substrate as shown below




Heat: 200 – 2200°C

**Figure 6.** Chemical vapour deposition reactor

In a tungsten CVD reactor system, it has been observed that the temperature of the heated wafer (substrate) can be a strong function of the gas composition when all other factors are kept constant. The table below shows the wafer temperature as a function of gas composition. Using least squares optimization fit the data to the linear equation

$$T = ax + b$$

where T is the wafer temperature, and x represents the $H_2$ mole fraction in a hydrogen-nitrogen gas mixture.

| $H_2$, mole fraction | *T* (K) |
|---|---|
| 1.0 | 553.33 |
| 0.8 | 577.33 |
| 0.6 | 602.33 |
| 0.4 | 626.67 |
| 0.0 | 672.67 |

**Question 1.23**
Consider a batch reactor with a single first-order reaction, $A \to B$. Data from the reactor is given in the Table below

**Concentration as a function of time**

| time, min | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| $C_A$, kgmol/m$^3$ | 8.47 | 5.00 | 2.95 | 1.82 | 1.05 | 0.71 |

The model is:

$$\frac{dC_A}{dt} = -kC_A$$

where $C_A$ is the concentration of $A$, $k$ is the rate constant, and $t$ is time.
solving the above by separating variables and integrating gives:

$$\frac{dC_A}{C_A} = -kdt$$

$$\ln C_A = \ln C_{Ao} - kt$$

Using the experimental data given above and a linear expression of the form $y = \beta_0 + \beta_1 x$ for the best fit line, obtain the parameters, $C_{Ao}$ and $k$ for the model. Compare the experimental data with your best fit line (model)

**Question 1.24**
The Arrhenius rate expression is used to find reaction rate constants as a function of temperature:

$$k = Ae^{-E/RT}$$

Taking the natural log (In) of each side of the Arrhenius rate expression, gives:

$$\ln k - \ln A - (E/R)(1/T)$$

where R is the ideal gas constant (1.987 cal/gmol K).

For the first order reaction given in Question 1.16, the rate constants as a function of temperature is shown below:

| $k$, min$^{-1}$ | 0.026 | 0.062 | 0.108 | 0.213 | 0.43 |
|---|---|---|---|---|---|
| $T$,K | 313 | 319 | 323 | 328 | 333 |

Find A and E using least squares analysis (show units). Compare model and experiment by
(i) plotting ln k versus 1/$T$ and
(ii) $k$ versus $T$.

**Question 1.25**

The growth rate expression for a biochemical reaction, using a Monod model, is:

$$\mu = \frac{\mu_{\max} x}{k_m + x}$$

where $\mu$ is the specific growth rate, $\mu_{max}$ and $k_m$ are parameters, and $x$ is the substrate concentration. The growth rate relationship can be rearranged to:

$$\frac{1}{\mu} = \left(\frac{1}{\mu_{\max}}\right) + \left(\frac{k_m}{\mu_{\max}}\right)\left(\frac{1}{x}\right)$$

Data for a particular reactor are shown below. Use least squares method to solve for the parameters ($\mu_{max}$ and $k_m$).

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| μ, $hr^{-1}$ | 0.25 | 0.31 | 0.36 | 0.43 | 0.45 | 0.47 | 0.50 | 0.52 |
| $x$, g/litre | 0.1 | 0.15 | 0.25 | 0.50 | 0.75 | 1.00 | 1.50 | 3.00 |

**Question 1.26**

Using a substrate inhibition model for the growth rate expression for a biochemical reaction gives

$$\mu = \frac{\mu_{\max} x}{k_m + x + k_1 x^2}$$

where the parameters are as defined in question 1.18 The new growth rate relationship when rearranged gives:

$$\frac{1}{\mu} = \left(\frac{k_1}{\mu_{\max}}\right) x + \left(\frac{k_m}{\mu_{\max}}\right)\left(\frac{1}{x}\right) + \left(\frac{1}{\mu_{\max}}\right)$$

Data for the particular reactor are shown below. Use least squares method to solve for the parameters ($\mu_{max}$, $k_m$, and $k_1$).

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| μ, $hr^{-1}$ | 0.24 | 0.27 | 0.34 | 0.35 | 0.35 | 0.34 | 0.33 | 0.22 |
| $x$, g/litre | 0.1 | 0.15 | 0.25 | 0.50 | 0.75 | 1.00 | 1.50 | 3.00 |

Note that:

$$\mathrm{Y} = \begin{bmatrix} 1/\mu_1 \\ 1/\mu_2 \\ \bullet \\ \bullet \\ 1/\mu_8 \end{bmatrix} \qquad \mathbf{X} = \begin{bmatrix} x_1 & 1/x_1 & 1 \\ x_2 & 1/x_2 & 1 \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ x_5 & 1/x_5 & 1 \end{bmatrix} \qquad \mathbf{B} = \begin{bmatrix} k_1/\mu_{\max} \\ k_m/\mu_{\max} \\ 1/\mu_{\max} \end{bmatrix}$$

Compare the model and experimental data by plotting $\mu$ vs. $x$.

# Grouping for PPS- 1

| Matric. No. | NAMES (SURNAME FIRST) | GRP No. |
|---|---|---|
| 170401513 | Adebayo Samuel | 1 |
| 160401039 | Adeniyi Adeyosola | |
| 160401067 | Akaforonye Johnpaul | |
| 170401520 | Chijioke Favour | |
| 160401033 | Ibrahim Ibrahim Christopher | |
| 150401018 | Musa Mohammed | |
| 160401008 | Obafemi Oluwadolapo | |
| 160401058 | Okafor Onyeka Peter | |
| 170401501 | Oladeji Ooreoluwa | |
| 160401017 | Onigemo Oluwatimilehin | |
| 160401018 | Abdul-Fatth Olaniyi Aamir | 2 |
| 170401521 | Adams Abdulsamad | |
| 160401025 | Adekanmbi Bisola | |
| 160401059 | Adekoya Kabir | |
| 160401024 | Idrees Idress Babatunde | |
| 160401041 | Ihade Kenneth | |
| 160401014 | Ofor Teresa Nneoma | |
| 160401068 | Ogunsina Oluwanifemi | |
| 150401054 | Ololade Kolade | |
| 170401505 | Oshakwuni Austin | |
| 160401001 | Agboola Damola Micheal | 3 |
| 160401021 | Dele-Safa Oluwatoba | |
| 170401507 | Goloba Sophiat | |
| 170401516 | Ibitoye Oluwajuwon | |
| 160401042 | Idris Idris Adeyemi | |
| 160401019 | Izuagbe Valerie | |
| 160401054 | Oladipo Abdul-Maleek | |
| 170401522 | Omo-Ojo Ekan | |
| 160401071 | Osunubi Oluwatobi | |
| 160401060 | Yaqub Abdulahhbasit | |
| 170401510 | Adewale Oluwatobi | 4 |
| 160401061 | Ayinde Sodiq | |
| 160401002 | Balogun Azeez Abayomi | |
| 160401044 | Idiege Idiege Peter | |
| 160401072 | Inaolaji Abidat | |
| 170401514 | Nwoye Chidinma | |
| 160401023 | Odejayi Olamide | |
| 170401509 | Ojeabulu Daniel | |
| 170401506 | Olalekan Funmilayo | |
| 170401523 | Opadotun Mofeoluwa | |

| | | |
|---|---|---|
| 170401502 | Adeyemi Esther | 5 |
| 160401073 | Agbeniyi Joshua | |
| 170401511 | Akinfoyewa Samuel | |
| 160401047 | Akpan Hope Nsibiet | |
| 160401028 | Ibitoye Rahman Oluwatobi | |
| 160401022 | Keshiro Monisola | |
| 160401012 | Ologunja Ebenezer | |
| 160401062 | Omoja Georgia | |
| 160401009 | Taiwo Raymond Olalekan | |
| 170401524 | Tortema Anuoluwapo | |
| 160401063 | Agbakoba Chukwunonso | 6 |
| 170401503 | Bright-Uteh Esther | |
| 170401527 | Chuks Enwerem Kelechi | |
| 160401070 | Ladipo Oluwafolaranmi | |
| 160401074 | Ogunnaike Olusola | |
| 160401010 | Ojukwu Ifeanyi | |
| 160401050 | Okonkwo Nnamdi Peter | |
| 160401030 | Olatunji Daniel | |
| 170401512 | Olowoporoku Adedoyin | |
| 160401005 | Oyebamiji Oluwaseyi | |
| 160401013 | Alebiosu Anthony | 7 |
| 160401052 | Anaje Daniel Ebube | |
| 170401515 | Bello Opeyemi | |
| 170401525 | Esanubong Itohowo | |
| 160401064 | Jegede Pelumi Emmanuel | |
| 170401504 | Merari Shalom | |
| 160401505 | Muoghara Augusta | |
| 160401031 | Nwokolo Fortune Chukwudalu | |
| 170401528 | Ogunrinde Oluwateniola | |
| 160401040 | Oyediran Toyese | |
| 160401056 | Adegbola Oluwatobi | 8 |
| 160401036 | Akinsanya Kofoworola | |
| 160401015 | Femi-Osofisan Tolulope | |
| 160401046 | Gbiri Oluwafemi | |
| 170401530 | Ghandhi Oceema | |
| 160401513 | Ilesanmi Samuel | |
| 170401517 | Khalejaiye Damola | |
| 160401007 | Mustapha Mubarak Ayomide | |
| 160401065 | Subair Husssein Kehinde | |
| 170401526 | Uwagbai Harriet | |
| 170401531 | Adegoke Jesulademi | 9 |
| 160401029 | Adekogbe Fortune Tolulope | |
| 160401057 | Atinmo Oyindamola | |
| 160401003 | Kareem Wajud Babatunde | |
| 160401535 | Obinna Michael | |
| 160401066 | Ojo Micheal Oluwatobi | |
| 160401016 | Ojure Kamaldeen | |
| 170401518 | Salawu Opeyemi | |
| 160401037 | Shehu Faridah Titilayo | |
| 170401531 | Adegoke Jesulademi | |